INVENTOR SEARCH

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=> fil capl
FILE 'CAPLUS' ENTERED AT 14:33:03 ON 01 FEB 2008
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FILE COVERS 1907 - 1 Feb 2008  VOL 148 ISS 6
FILE LAST UPDATED: 31 Jan 2008  (20080131/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> => d que nos l41
L3            39 SEA FILE=REGISTRY ABB=ON  (116046-53-8/BI OR 128095-14-7/BI OR
                 1583-88-6/BI OR 1655-07-8/BI OR 21615-34-9/BI OR 22396-14-1/BI
                 OR 404-70-6/BI OR 51756-10-6/BI OR 52721-69-4/BI OR 5538-51-2/B
                 I OR 607-97-6/BI OR 609-14-3/BI OR 611-10-9/BI OR 64-04-0/BI
                 OR 780771-35-9/BI OR 780771-36-0/BI OR 780771-37-1/BI OR
                 780771-38-2/BI OR 780771-39-3/BI OR 780771-40-6/BI OR 780771-41
                 -7/BI OR 780771-42-8/BI OR 780771-43-9/BI OR 780771-44-0/BI OR
                 780771-45-1/BI OR 780771-46-2/BI OR 780771-47-3/BI OR 780771-48
                 -4/BI OR 780771-49-5/BI OR 780771-50-8/BI OR 780771-51-9/BI OR
                 780771-52-0/BI OR 780771-54-2/BI OR 780771-55-3/BI OR 780771-56
                 -4/BI OR 780771-57-5/BI OR 780771-58-6/BI OR 85796-29-8/BI OR
                 916335-88-1/BI)
L38            1 SEA FILE=CAPLUS ABB=ON  US2006-551920/AP
L40        12524 SEA FILE=CAPLUS ABB=ON  L3
L41            1 SEA FILE=CAPLUS ABB=ON  L40 AND L38


=> fil casre; d que nos l29
FILE 'CASREACT' ENTERED AT 14:34:13 ON 01 FEB 2008
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FILE CONTENT:1840 - 26 Jan 2008 VOL 148 ISS 5

New CAS Information Use Policies, enter HELP USAGETERMS for details.
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*************************************************************
*                                                           *
*     CASREACT now has more than 13.8 million reactions     *
*                                                           *
*************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.


L1              STR
L2       448706 SEA FILE=REGISTRY SSS FUL L1
L4        46492 SEA FILE=REGISTRY ABB=ON  L2 AND CASREACT/LC
L5        10919 SEA FILE=CASREACT ABB=ON  L4
L8              STR
L11        1257 SEA FILE=CASREACT SUB=L5 SSS FUL L8 ( 11881 REACTIONS)
L21 (        29)SEA FILE=CASREACT ABB=ON  SHCHERBAKOVA I?/AU
L22 (         0)SEA FILE=CASREACT ABB=ON  BALANDRIA M?/AU
L23 (       108)SEA FILE=CASREACT ABB=ON  HUANG G?/AU
L24 (         5)SEA FILE=CASREACT ABB=ON  GEOFFROY O?/AU
L25 (       117)SEA FILE=CASREACT ABB=ON  FOX J?/AU
L26 (        51)SEA FILE=CASREACT ABB=ON  NAIR S?/AU
L27 (         7)SEA FILE=CASREACT ABB=ON  BALANDRIN M?/AU
L28           4 SEA FILE=CASREACT ABB=ON  (L21 AND (L22 OR L23 OR L24 OR L25
                OR L26 OR L27)) OR (L23 AND (L24 OR L25 OR L26 OR L27)) OR
                (L24 AND (L25 OR L26 OR L27)) OR (L25 AND (L26 OR L27)) OR
                (L26 AND L27)
L29           4 SEA FILE=CASREACT ABB=ON  L28 OR (L28 AND L11)


=> dup rem l41,l29
FILE 'CAPLUS' ENTERED AT 14:34:22 ON 01 FEB 2008
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FILE 'CASREACT' ENTERED AT 14:34:22 ON 01 FEB 2008
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PROCESSING COMPLETED FOR L41
PROCESSING COMPLETED FOR L29
L42           4 DUP REM L41 L29 (1 DUPLICATE REMOVED)
                ANSWER '1' FROM FILE CAPLUS
                ANSWERS '2-4' FROM FILE CASREACT

=> d ibib abs hitstr 1; d iall 2-4

L42  ANSWER 1 OF 4  CAPLUS  COPYRIGHT 2008 ACS on STN  DUPLICATE 1
ACCESSION NUMBER:         2004:902339  CAPLUS  Full-text
DOCUMENT NUMBER:          141:379934
TITLE:                    Preparation of 2,3,5,6-tetrasubstituted
                          3H-pyrimidin-4-ones via cyclization of carboxamides.
INVENTOR(S):              Shcherbakova, Irina; Balandrin, Manuel; Huang,
                          Guangfei; Geoffroy, Otto; Fox, John; Nair, Satheesh K.
PATENT ASSIGNEE(S):       NPS Pharmaceuticals, Inc., USA
SOURCE:                   PCT Int. Appl., 33 pp.
```

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092121	A2	20041028	WO 2004-US10639	20040407
WO 2004092121	A3	20050414		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1613606	A2	20060111	EP 2004-749815	20040407
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2006522160	T	20060928	JP 2006-509759	20040407
US 2007161792	A1	20070712	US 2006-551920	20061120 <--

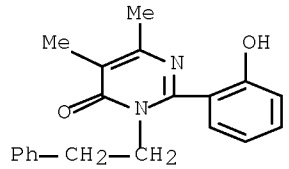
PRIORITY APPLN. INFO.:
US 2003-460859P P 20030407
US 2003-479323P P 20030618
WO 2004-US10639 W 20040407

OTHER SOURCE(S): CASREACT 141:379934; MARPAT 141:379934

AB The title process is claimed. Thus, 3-(2-acetoxybenzoylamino)-2-methylbut- 2-enoic acid phenethylamide (preparation given) was refluxed overnight with KOH in EtOH/H2O to give 37% 2-(2-hydroxyphenyl)-5,6-dimethyl-3-phenethyl-3H-pyrimidin-4-one.

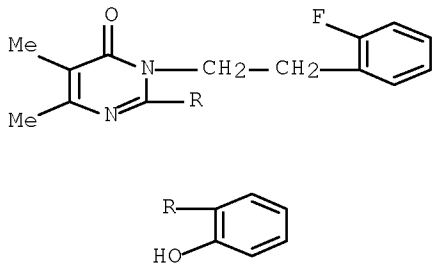
IT 780771-35-9P 780771-40-6P 780771-41-7P
780771-42-8P 780771-43-9P 780771-44-0P
780771-45-1P 780771-46-2P 780771-47-3P
780771-48-4P 780771-51-9P 780771-52-0P
780771-54-2P 780771-55-3P 780771-56-4P
780771-57-5P 780771-58-6P 916335-88-1P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of tetrasubstituted pyrimidinones via cyclization of carboxamides)

RN 780771-35-9 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5,6-dimethyl-3-(2-phenylethyl)- (CA INDEX NAME)



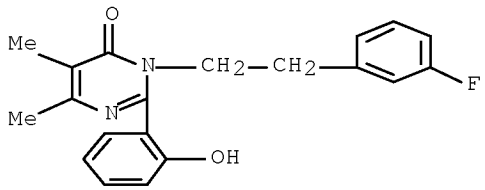
RN 780771-40-6 CAPLUS

CN 4(3H)-Pyrimidinone, 3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl- (CA INDEX NAME)



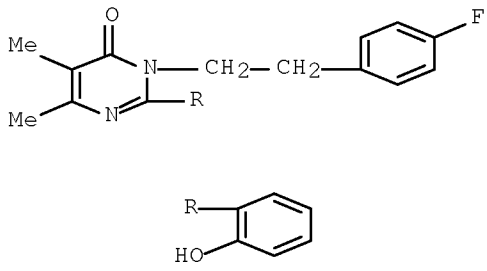
RN 780771-41-7 CAPLUS

CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl- (CA INDEX NAME)



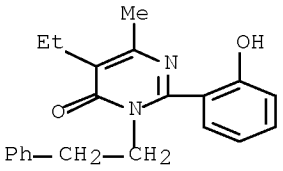
RN 780771-42-8 CAPLUS

CN 4(3H)-Pyrimidinone, 3-[2-(4-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl- (CA INDEX NAME)

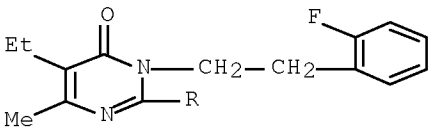


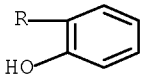
RN 780771-43-9 CAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)

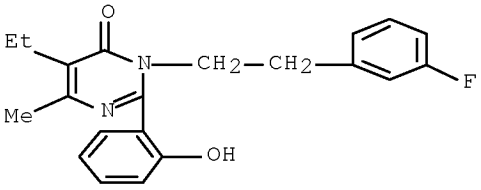


RN 780771-44-0 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)

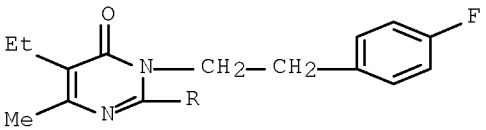


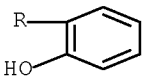


RN 780771-45-1 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



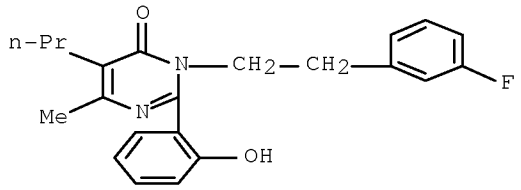
RN 780771-46-2 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(4-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



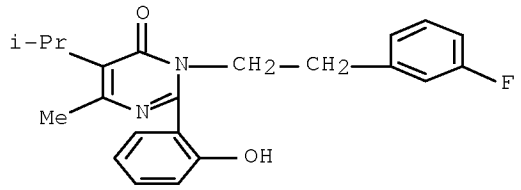


RN 780771-47-3 CAPLUS

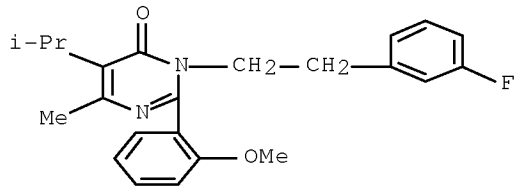
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-propyl- (CA INDEX NAME)



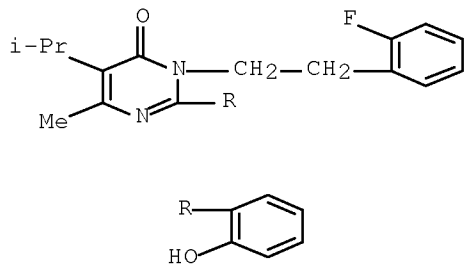
RN 780771-48-4 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



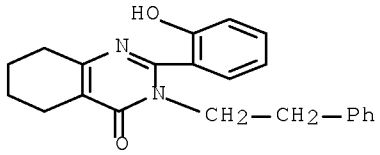
RN 780771-51-9 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-methoxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



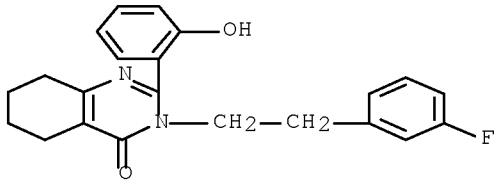
RN 780771-52-0 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



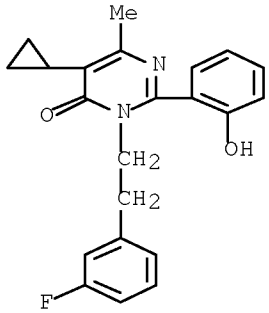
RN 780771-54-2 CAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



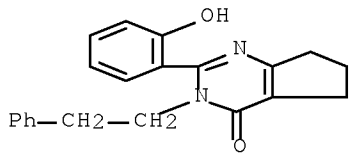
RN 780771-55-3 CAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)- (CA INDEX NAME)



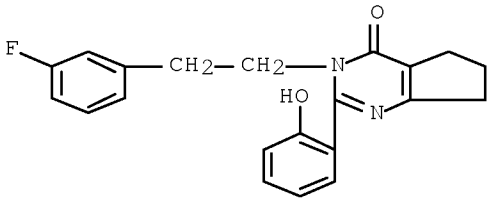
RN 780771-56-4 CAPLUS
CN 4(3H)-Pyrimidinone, 5-cyclopropyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



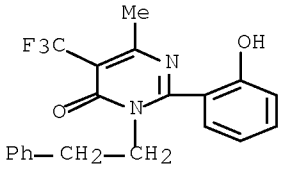
RN 780771-57-5 CAPLUS
CN 4H-Cyclopentapyrimidin-4-one, 3,5,6,7-tetrahydro-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (9CI) (CA INDEX NAME)



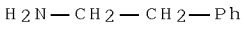
RN 780771-58-6 CAPLUS
CN 4H-Cyclopentapyrimidin-4-one, 3-[2-(3-fluorophenyl)ethyl]-3,5,6,7-tetrahydro-2-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)



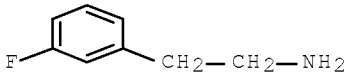
RN 916335-88-1 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(trifluoromethyl)- (CA INDEX NAME)



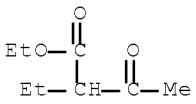
IT 64-04-0, Phenethylamine 404-70-6, 3-Fluorophenethylamine 607-97-6, Ethyl 2-ethyl-3-oxobutyrate 609-14-3, Ethyl 2-methyl-3-oxobutyrate 611-10-9, Ethyl 2-oxocyclopentanecarboxylate 1583-88-6, 4-Fluorophenethylamine 1655-07-8, Ethyl 2-oxocyclohexanecarboxylate 5538-51-2 21615-34-9 22396-14-1 51756-10-6 52721-69-4, 2-Fluorophenethylamine 116046-53-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of tetrasubstituted pyrimidinones via cyclization of carboxamides)
RN 64-04-0 CAPLUS
CN Benzeneethanamine (CA INDEX NAME)



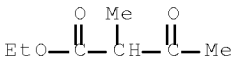
RN 404-70-6 CAPLUS
CN Benzeneethanamine, 3-fluoro- (CA INDEX NAME)



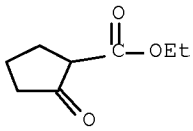
RN 607-97-6 CAPLUS
CN Butanoic acid, 2-ethyl-3-oxo-, ethyl ester (CA INDEX NAME)



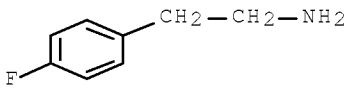
RN 609-14-3 CAPLUS
CN Butanoic acid, 2-methyl-3-oxo-, ethyl ester (CA INDEX NAME)



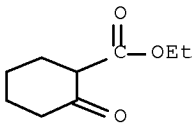
RN 611-10-9 CAPLUS
CN Cyclopentanecarboxylic acid, 2-oxo-, ethyl ester (CA INDEX NAME)



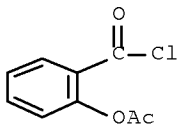
RN 1583-88-6 CAPLUS
CN Benzeneethanamine, 4-fluoro- (CA INDEX NAME)



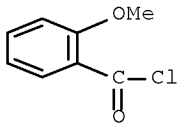
RN 1655-07-8 CAPLUS
CN Cyclohexanecarboxylic acid, 2-oxo-, ethyl ester (CA INDEX NAME)



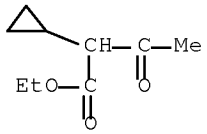
RN 5538-51-2 CAPLUS
CN Benzoyl chloride, 2-(acetyloxy)- (CA INDEX NAME)



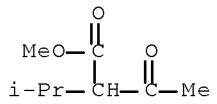
RN 21615-34-9 CAPLUS
CN Benzoyl chloride, 2-methoxy- (CA INDEX NAME)



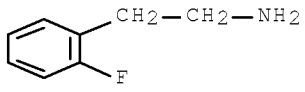
RN 22396-14-1 CAPLUS
CN Cyclopropaneacetic acid, α-acetyl-, ethyl ester (CA INDEX NAME)



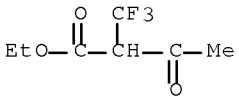
RN 51756-10-6 CAPLUS
CN Butanoic acid, 2-acetyl-3-methyl-, methyl ester (CA INDEX NAME)



RN 52721-69-4 CAPLUS
CN Benzeneethanamine, 2-fluoro- (CA INDEX NAME)



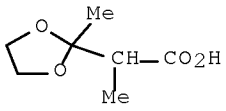
RN 116046-53-8 CAPLUS
CN Butanoic acid, 3-oxo-2-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)



IT 85796-29-8P 128095-14-7P 780771-36-0P
780771-37-1P 780771-38-2P 780771-39-3P
780771-49-5P, 3-Amino-2-isopropylbut-3-enoic acid methyl ester
780771-50-8P, 2-Isopropyl-3-(2-methoxybenzoylamino)but-3-enoic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tetrasubstituted pyrimidinones via cyclization of carboxamides)

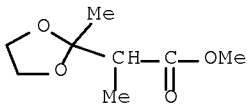
RN 85796-29-8 CAPLUS

CN 1,3-Dioxolane-2-acetic acid, α,2-dimethyl- (CA INDEX NAME)



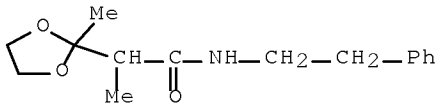
RN 128095-14-7 CAPLUS

CN 1,3-Dioxolane-2-acetic acid, α,2-dimethyl-, methyl ester (CA INDEX NAME)



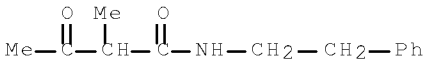
RN 780771-36-0 CAPLUS

CN 1,3-Dioxolane-2-acetamide, α,2-dimethyl-N-(2-phenylethyl)- (CA INDEX NAME)

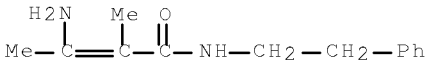


RN 780771-37-1 CAPLUS

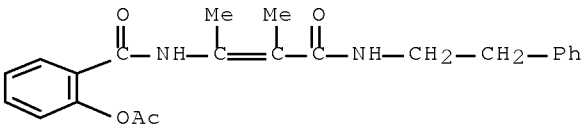
CN Butanamide, 2-methyl-3-oxo-N-(2-phenylethyl)- (CA INDEX NAME)



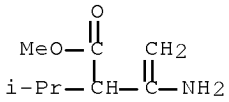
RN 780771-38-2 CAPLUS
CN 2-Butenamide, 3-amino-2-methyl-N-(2-phenylethyl)- (CA INDEX NAME)



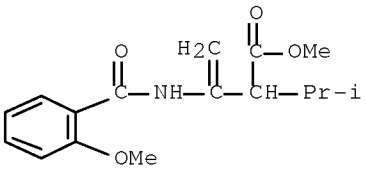
RN 780771-39-3 CAPLUS
CN Benzamide, 2-(acetyloxy)-N-[1,2-dimethyl-3-oxo-3-[(2-phenylethyl)amino]-1-propenyl]- (9CI) (CA INDEX NAME)



RN 780771-49-5 CAPLUS
CN 3-Butenoic acid, 3-amino-2-(1-methylethyl)-, methyl ester (CA INDEX NAME)

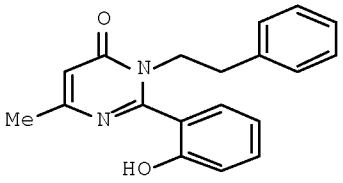


RN 780771-50-8 CAPLUS
CN 3-Butenoic acid, 3-[(2-methoxybenzoyl)amino]-2-(1-methylethyl)-, methyl ester (CA INDEX NAME)



L42 ANSWER 2 OF 4 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 143:59927 CASREACT Full-text
TITLE: Design, new synthesis, and calcilytic activity of substituted 3H-pyrimidin-4-ones
AUTHOR(S): Shcherbakova, Irina; Huang, Guangfei ; Geoffroy, Otto J.; Nair, Satheesh

K.; Swierczek, Krzysztof; Balandrin, Manuel F.; Fox, John; Heaton, William L.; Conklin, Rebecca L.
CORPORATE SOURCE: Drug Discovery, NPS Pharmaceuticals, Inc., Salt Lake City, UT, 84108, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(10), 2537-2540
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
GRAPHIC IMAGE:



I

ABSTRACT:
Design, synthesis, structure-activity relationship studies and calcium receptor antagonist (calcilytic) properties of 3H-pyrimidin-4-ones, e.g., I, are described. The pyrimidinones were synthesized by multistep procedures.

SUPPL. TERM: keto ester amidine heterocyclization; pyrimidinone prepn calcilytic
INDEX TERM: Amines, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(aralkyl; preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)
INDEX TERM: Receptors
ROLE: BSU (Biological study, unclassified); BIOL (Biological study)
(calcium; preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)
INDEX TERM: Carboxylic acids, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(oxo, esters; preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)
INDEX TERM: Heterocyclization
(preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from

hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

INDEX TERM: Structure-activity relationship (receptor-binding, CaR; preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

INDEX TERM: 780771-32-6P 780771-33-7P 780771-34-8P 780771-35-9P
780771-41-7P 780771-43-9P 780771-44-0P 780771-47-3P
780771-48-4P 780771-53-1P 780771-54-2P 780771-55-3P
780771-56-4P 780771-57-5P 780771-58-6P
ROLE: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

INDEX TERM: 64-04-0, 2-Phenylethylamine 105-45-3, Methyl acetoacetate
344-00-3 404-70-6, 2-(3-Fluorophenyl)ethylamine 607-97-6
609-14-3 611-10-9 611-20-1, 2-Hydroxybenzonitrile
1522-46-9 1540-28-9 1655-07-8 5538-51-2,
2-Acetoxybenzoyl chloride 22396-14-1 52721-69-4,
2-(2-Fluorophenyl)ethylamine
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

INDEX TERM: 4746-93-4P 7646-61-9P 13747-72-3P 23153-73-3P
26384-76-9P 27773-09-7P 27773-10-0P 38853-85-9P
85796-29-8P 90647-54-4P 130625-27-3P 610754-95-5P
751428-10-1P 780771-36-0P 780771-37-1P 780771-38-2P
780771-39-3P 854132-93-7P 854132-94-8P 854132-95-9P
854132-96-0P 854132-97-1P 854132-98-2P 854132-99-3P
854133-00-9P 854133-01-0P 854133-02-1P 854133-03-2P
854133-04-3P 854133-05-4P 854133-06-5P 854133-07-6P
854133-08-7P 854133-09-8P 854133-10-1P 854133-11-2P
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854133-44-1P 854133-45-2P 854133-46-3P 854133-47-4P
854133-48-5P 854133-49-6P 854133-50-9P 854133-51-0P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S): (1) Altmann, E; WO 2004/056365 A2 CAPLUS
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(19) Shcherbakova, I; WO 2004/092120 A2 CAPLUS
(20) Shcherbakova, I; WO 2004/092121 A2 CAPLUS
(21) Shcherbakova, I; 2004 CAPLUS
(22) Shcherbakova, I; 2004 CAPLUS
(23) Shcherbakova, I; 2004 CAPLUS
(24) Shcherbakova, I; Bioorg Med Chem Lett 2005, V15, P1557 CAPLUS
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=> d ibib abs ind 3-4

L42 ANSWER 3 OF 4 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 142:348143 CASREACT Full-text
TITLE: 3H-Quinazolin-4-ones as a new calcilytic template for the potential treatment of osteoporosis
AUTHOR(S): Shcherbakova, Irina; Balandrin, Manuel F.; Fox, John; Ghatak, Anjan; Heaton, William L.; Conklin, Rebecca L.
CORPORATE SOURCE: Drug Discovery, NPS Pharmaceuticals, Inc., Salt Lake City, UT, 84108, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(6), 1557-1560
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Structure-activity relationship studies, focused on identification of the active pharmacophore fragments in a single high-throughput screening calcilytic hit, resulted in the discovery of potent calcium receptor antagonists, substituted 3H-quinazolin-4-ones.
CC 1-3 (Pharmacology)
Section cross-reference(s): 28
ST quinazolinone deriv prepn structure osteoporosis
IT Bone resorption inhibitors
Osteoporosis
Structure-activity relationship
(3H-quinazolin-4-ones preparation and structure-related potential for

osteoporosis treatment)
IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(calcium; 3H-quinazolin-4-ones preparation and structure-related potential for osteoporosis treatment)
IT 7440-70-2, Calcium, biological studies 9002-64-6, Parathyroid hormone
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(3H-quinazolin-4-ones preparation and structure-related potential for osteoporosis treatment)
IT 691378-86-6P 849233-11-0P 849233-12-1P
RL: BYP (Byproduct); PREP (Preparation)
(3H-quinazolin-4-ones preparation and structure-related potential for osteoporosis treatment)
IT 312277-73-9P 450378-70-8P 489416-64-0P 691378-17-3P 691378-21-9P
691378-24-2P 691378-25-3P 691378-26-4P 691378-28-6P 691378-34-4P
691378-45-7P 691378-46-8P 691378-47-9P 691378-49-1P 691378-50-4P
691378-53-7P 691378-54-8P 691378-65-1P 691378-94-6P 849233-10-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(3H-quinazolin-4-ones preparation and structure-related potential for osteoporosis treatment)
IT 328540-74-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3H-quinazolin-4-ones preparation and structure-related potential for osteoporosis treatment)
IT 64-04-0, Benzeneethanamine 89-77-0 98-88-4, Benzoyl chloride
100-07-2 118-92-3 393-52-2 404-70-6 434-76-4 446-08-2 446-32-2
635-21-2 825-22-9 1711-05-3 1711-07-5 2941-78-8 4389-45-1
4389-50-8 5538-51-2 13078-79-0 16446-73-4 21615-34-9 27914-73-4
37785-02-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(3H-quinazolin-4-ones preparation and structure-related potential for osteoporosis treatment)
IT 1022-46-4P 18595-84-1P 18600-55-0P 35673-24-6P 60681-96-1P
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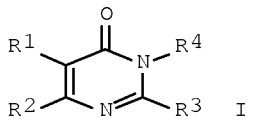
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(3H-quinazolin-4-ones preparation and structure-related potential for osteoporosis treatment)
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 4 OF 4 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 141:366249 CASREACT Full-text
TITLE: Preparation of pyrimidinone compounds as calcilytics
INVENTOR(S): Shcherbakova, Irina V.; Balandrin, Manuel F.; Huang, Guangfei; Geoffroy, Otto; Fox, John; Marquis, Robert; Yamashita, Dennis Shinji; Luengo, Juan; Wang, Wenyong
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA; Glaxosmithkline
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092120	A2	20041028	WO 2004-US10638	20040407
WO 2004092120	A3	20050414		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004230903	A1	20041028	AU 2004-230903	20040407
CA 2521129	A1	20041028	CA 2004-2521129	20040407
EP 1615897	A2	20060118	EP 2004-749814	20040407
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1835928	A	20060920	CN 2004-80009255	20040407
JP 2006522159	T	20060928	JP 2006-509758	20040407
MX 2005PA10683	A	20060801	MX 2005-PA10683	20051004
US 2007197555	A1	20070823	US 2006-552363	20061120
PRIORITY APPLN. INFO.:			US 2003-460859P	20030407
			US 2003-479323P	20030618
			WO 2004-US10638	20040407

OTHER SOURCE(S): MARPAT 141:366249
GI



I

AB Title compds. I [R1-2 = H, halo, CN, CF3, etc.; R3 = aryl; R4 = H, alkyl, etc.] are prepared For instance, 2-(2-Hydroxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one is prepared from o-hydroxybenzonitrile, acetyl chloride and Me acetoacetate. Compds. of the invention have IC50 values < 30 μM in a calcium receptor inhibition assay. I are useful for the treatment of abnormal bone or mineral homeostasis.

IC ICM C07D
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
ST pyrimidinone calcilytic calcium receptor antagonist prepn
IT Bone, disease
(Paget's; preparation of pyrimidinone compds. as calcilytics)
IT Homeostasis
(bone or mineral disorders; preparation of pyrimidinone compds. as calcilytics)
IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)

(calcium; preparation of pyrimidinone compds. as calcilytics)
IT Bone, neoplasm
Sarcoma
(osteosarcoma; preparation of pyrimidinone compds. as calcilytics)
IT Antirheumatic agents
Human
Osteoarthritis
Osteoporosis
Periodontium, disease
Rheumatoid arthritis
Wound healing
(preparation of pyrimidinone compds. as calcilytics)
IT 7440-70-2, Calcium, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hypercalcemia; preparation of pyrimidinone compds. as calcilytics)
IT 9002-64-6, Parathyroid hormone
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of pyrimidinone compds. as calcilytics)
IT 780771-43-9P, 5-Ethyl-2-(2-hydroxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one 780771-51-9P, 3-[2-(3-Fluorophenyl)ethyl]-5-isopropyl-2-(2-methoxyphenyl)-6-methyl-3H-pyrimidin-4-one
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrimidinone compds. as calcilytics)
IT 780771-32-6P, 2-(2-Hydroxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one 780771-33-7P, 3-[2-(2-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-34-8P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-35-9P, 2-(2-Hydroxyphenyl)-5,6-dimethyl-3-phenethyl-3H-pyrimidin-4-one 780771-40-6P, 3-[2-(2-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl-3H-pyrimidin-4-one 780771-41-7P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl-3H-pyrimidin-4-one 780771-42-8P, 3-[2-(4-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl-3H-pyrimidin-4-one 780771-44-0P, 5-Ethyl-3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-45-1P 780771-46-2P, 5-Ethyl-3-[2-(4-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-47-3P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-propyl-3H-pyrimidin-4-one 780771-48-4P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5-isopropyl-6-methyl-3H-pyrimidin-4-one 780771-52-0P, 3-[2-(2-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5-isopropyl-6-methyl-3H-pyrimidin-4-one 780771-53-1P, 2-(2-Hydroxyphenyl)-5-methyl-3-phenethyl-6-trifluoromethyl-3H-pyrimidin-4-one 780771-54-2P, 2-(2-Hydroxyphenyl)-3-phenethyl-5,6,7,8-tetrahydro-3H-quinazolin-4-one 780771-55-3P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6,7,8-tetrahydro-3H-quinazolin-4-one 780771-56-4P, 5-Cyclopropyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-57-5P, 2-(2-Hydroxyphenyl)-3-phenethyl-3,5,6,7-tetrahydrocyclopenta[1,2-d]pyrimidin-4-one 780771-58-6P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-3,5,6,7-tetrahydrocyclopenta[1,2-d]pyrimidin-4-one 780771-59-7P, 5-Ethyl-2-(2-methoxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one 780771-60-0P, 2-(5-Chloro-2-hydroxypyridin-3-yl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-62-2P, 5-Ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-64-4P, 5-Ethyl-2-(5-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-65-5P, 5-Ethyl-2-(2-fluoro-6-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-67-7P, 2-(5-Chloro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-68-8P,

2-(5-Bromo-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-69-9P, 5-Ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-3-isopropylphenyl)-6-methyl-3H-pyrimidin-4-one 780771-71-3P, 2-(3,5-Dibromo-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-72-4P, 5-Ethyl-2-(3-chloro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-74-6P, 5-Ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-3-methylphenyl)-6-methyl-3H-pyrimidin-4-one 780771-75-7P, 2-(4-Chloro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-76-8P, 5-Ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-4-methoxyphenyl)-6-methyl-3H-pyrimidin-4-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinone compds. as calcilytics)

IT 64-04-0, Phenethylamine 75-36-5, Acetyl chloride 100-58-3, Phenylmagnesium bromide 105-45-3, Methyl acetoacetate 404-70-6, 2-(3-Fluorophenyl)ethylamine 607-97-6, 2-Ethyl-3-oxobutanoic acid ethyl ester 609-14-3, 2-Methyl-3-oxobutyric acid ethyl ester 611-10-9, 2-Oxocyclopentanecarboxylic acid ethyl ester 611-20-1, o-Hydroxybenzonitrile 1522-46-9, 2-Isopropyl-3-oxobutanoic acid ethyl ester 1540-28-9, 2-Propyl-3-oxobutanoic acid ethyl ester 1583-88-6, 4-Fluorophenethylamine 1655-07-8, 2-Oxocyclohexanecarboxylic acid ethyl ester 5485-91-6, Acetic acid 4-bromo-2-chlorocarbonylphenyl ester 5538-51-2, Acetic acid 2-chlorocarbonylphenyl ester 5538-52-3, Acetic acid 2-chlorocarbonyl-4-fluorophenyl ester 5538-53-4, Acetic acid 4-chloro-2-chlorocarbonylphenyl ester 17094-21-2, 2-Methyl-3-oxobutanoic acid methyl ester 19202-27-8, Acetic acid 2-chlorocarbonylmethoxyphenyl ester 21615-34-9 22396-14-1, 2-Cyclopropyl-3-oxobutanoic acid ethyl ester 26384-76-9 27893-05-6, Acetic acid 2-chlorocarbonyl-6-methylphenyl ester 52721-69-4, 2-(2-Fluorophenyl)ethylamine 54223-78-8 54551-50-7, Acetic acid 5-chloro-2-chlorocarbonylphenyl ester 116046-53-8, 2-Trifluoromethyl-3-oxobutanoic acid ethyl ester 780771-61-1, 2-Acetoxy-5-chloronicotinoyl chloride 780771-63-3, Acetic acid 2-chlorocarbonyl-6-fluorophenyl ester 780771-66-6, Acetic acid 2-chlorocarbonyl-3-fluorophenyl ester 780771-70-2, Acetic acid 2-chlorocarbonyl-6-isopropylphenyl ester 780771-73-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinone compds. as calcilytics)

IT 27773-09-7P, 2-(2-Methyl-[1,3]dioxolan-2-yl)propionic acid ethyl ester 61636-46-2P 85796-29-8P, 2-(2-Methyl-[1,3]dioxolan-2-yl)propionic acid 780771-36-0P, 2-(2-Methyl-[1,3]dioxolan-2-yl)-N-phenethylpropaneamide 780771-37-1P, 2-Methyl-3-oxo-N-phenethylbutyramide 780771-38-2P, 3-Amino-2-methylbut-2-enoic acid phenethylamide 780771-39-3P, Acetic acid 2-((1-methyl-2-((phenethyl)carbamoyl)propenyl)carbamoyl)phenyl ester 780771-49-5P, 3-Amino-2-isopropylbut-3-enoic acid methyl ester 780771-50-8P, 2-Isopropyl-3-(2-methoxybenzoylamino)but-3-enoic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidinone compds. as calcilytics)

STRUCTURE SEARCH

```
=> fil casre; d stat que l20;s l20 not l29; fil reg; d stat que l36; fil capl; d
que nos l37; s l37 not l41
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FILE CONTENT:1840 - 26 Jan 2008 VOL 148 ISS 5

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************************************************************
*                                                          *
*     CASREACT now has more than 13.8 million reactions    *
*                                                          *
************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
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This file contains CAS Registry Numbers for easy and accurate substance
identification.


L1              STR
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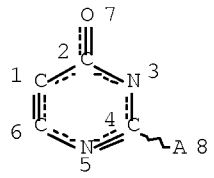


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NODE ATTRIBUTES:
NSPEC   IS RC     AT   8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   8

STEREO ATTRIBUTES: NONE
L2       448706 SEA FILE=REGISTRY SSS FUL L1
L4        46492 SEA FILE=REGISTRY ABB=ON  L2 AND CASREACT/LC
L5        10919 SEA FILE=CASREACT ABB=ON  L4
L8              STR
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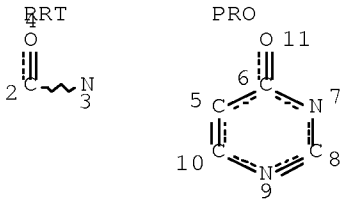

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

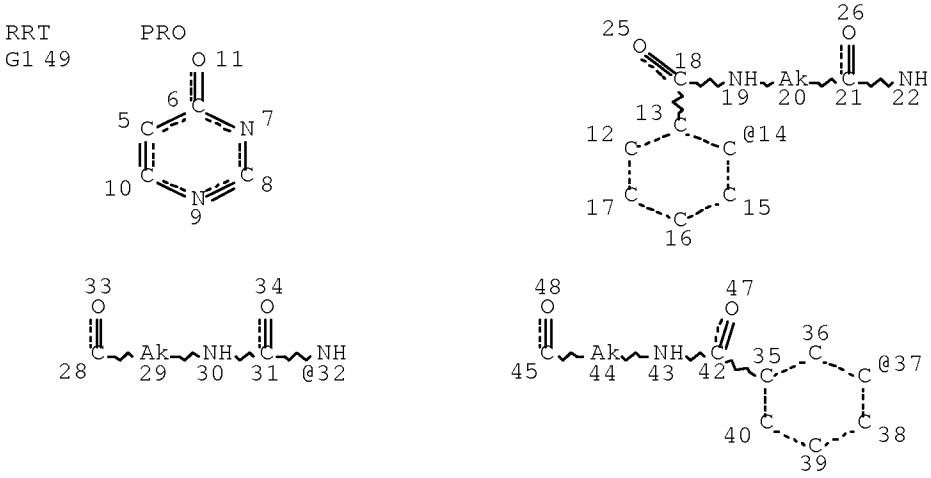
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

****MAPPINGS****

NOD	SYM	ROL	NOD	SYM	ROL
2	C	RRT	6	C	PRO
3	N	RRT	7	N	PRO
4	O	RRT	11	O	PRO
6	C	PRO	2	C	RRT
7	N	PRO	3	N	RRT
11	O	PRO	4	O	RRT

L11 1257 SEA FILE=CASREACT SUB=L5 SSS FUL L8 (11881 REACTIONS)
L12 1118 SEA FILE=CASREACT ABB=ON L11/COMPLETE
L13 902 SEA FILE=CASREACT ABB=ON L12 AND (PY<2004 OR AY<2004 OR PRY<2004)
L16 STR



VAR G1=14/32/37
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 20
CONNECT IS E2 RC AT 29
CONNECT IS E2 RC AT 44
DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 40

STEREO ATTRIBUTES: NONE
L19 22 SEA FILE=CASREACT SUB=L11 SSS FUL L16 (56 REACTIONS)
L20 16 SEA FILE=CASREACT ABB=ON L13 AND L19

L43 14 L20 NOT L29

FILE 'REGISTRY' ENTERED AT 14:37:45 ON 01 FEB 2008
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STRUCTURE FILE UPDATES: 31 JAN 2008 HIGHEST RN 1001228-41-6
DICTIONARY FILE UPDATES: 31 JAN 2008 HIGHEST RN 1001228-41-6

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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REGISTRY includes numerically searchable data for experimental and
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experimental property data in the original document. For information
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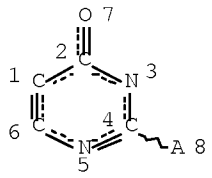
http://www.cas.org/support/stngen/stndoc/properties.html

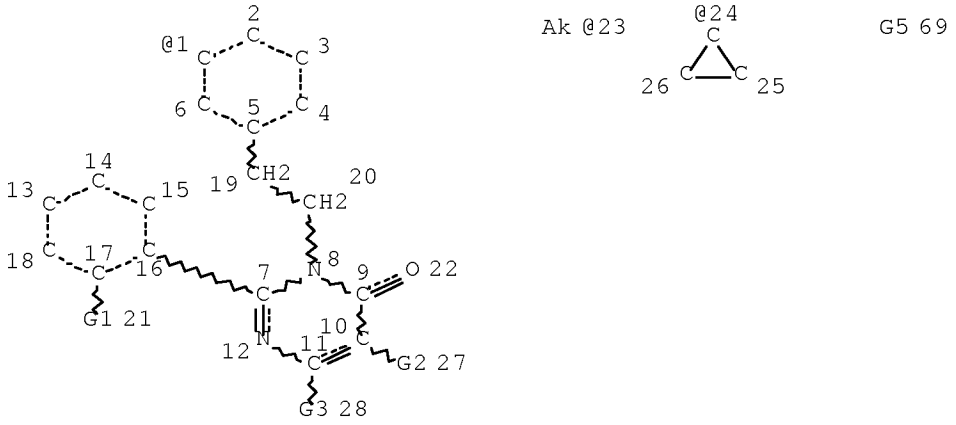
L1 STR



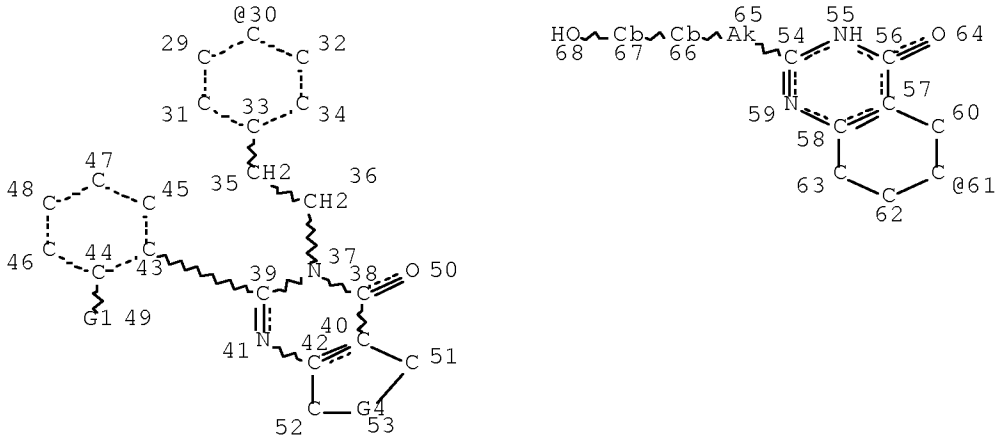
NODE ATTRIBUTES:
NSPEC IS RC AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L2 448706 SEA FILE=REGISTRY SSS FUL L1
L33 STR



Page 1-A



Page 2-A
VAR G1=OH/OME
VAR G2=23/24
VAR G3=23/CF3
REP G4=(1-2) C
VAR G5=1/61/30
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 23
CONNECT IS E2 RC AT 65
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY LOC UNS AT 66
GGCAT IS MCY LOC UNS AT 67
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 69

STEREO ATTRIBUTES: NONE

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L36          82 SEA FILE=REGISTRY SUB=L2 SSS FUL L33

100.0% PROCESSED   21805 ITERATIONS                              82 ANSWERS
SEARCH TIME: 00.00.01



FILE 'CAPLUS' ENTERED AT 14:37:45 ON 01 FEB 2008
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FILE COVERS 1907 - 1 Feb 2008  VOL 148 ISS 6
FILE LAST UPDATED: 31 Jan 2008  (20080131/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE


L1              STR
L2       448706 SEA FILE=REGISTRY SSS FUL L1
L33             STR
L36          82 SEA FILE=REGISTRY SUB=L2 SSS FUL L33
L37           5 SEA FILE=CAPLUS ABB=ON  L36/P



L44          4 L37 NOT L41

=> dup rem l43,l44
FILE 'CASREACT' ENTERED AT 14:38:00 ON 01 FEB 2008
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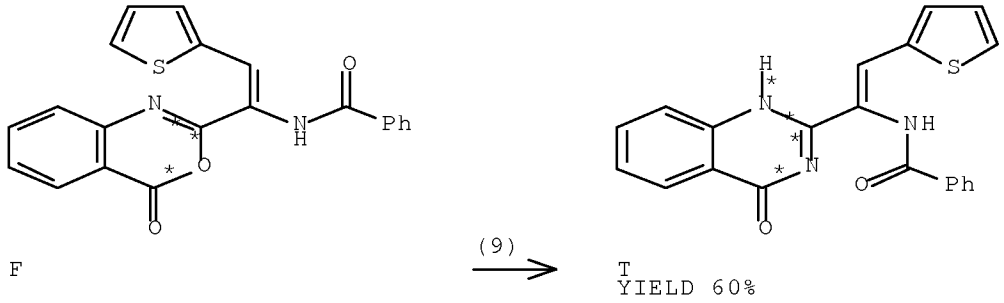
PROCESSING COMPLETED FOR L43
PROCESSING COMPLETED FOR L44
L45          18 DUP REM L43 L44 (0 DUPLICATES REMOVED)
                ANSWERS '1-14' FROM FILE CASREACT
                ANSWERS '15-18' FROM FILE CAPLUS

=> d ibib abs fhit 1-14; d ibib abs hitstr 15-18; fil hom
```

L45 ANSWER 1 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 134:86206 CASREACT Full-text
TITLE: The behaviour of some nucleophiles towards 2-[α-(benzoylamino)-β-(2-thienyl)vinyl]benzoxazin-4(3H)-one
AUTHOR(S): Guirguis, Dalal B.
CORPORATE SOURCE: Chemistry Department, Faculty of Science, Ain Shams University, Cairo, Egypt
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2000), 39B(4), 264-269
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication, CSIR
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 2-[α-(Benzoylamino)-β-thien-2-ylvinyl]benzoxazin-4(3H)-one (I) undergoes ring-opening on treatment with primary and secondary amines affording 2-[α-(benzoylamino)-β-thien-2- ylacrylamido]benzamides. Treatment of I with HCONH2 and N2H4.H2O at elevated temperature gives rise to quinazolinones. Interestingly, reaction of vicinal aminobenzyl alcs. with I yields the usual ring-opening products and unexpected 4-iminobenzoxazines.

RX(9) OF 80 ...F ===> T



RX(9) RCT F 318292-64-7

STAGE(1)
RGT U 75-12-7 Formamide
SOL 64-17-5 EtOH

STAGE(2)
SOL 7732-18-5 Water

PRO T 318292-72-7
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 2 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 138:106647 CASREACT Full-text

TITLE: Quinazolinones derived from N-(1,1-dimethylacetonyl)benzamide
AUTHOR(S): Usifoh, C. O.
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, University of Benin, Benin City, Nigeria
SOURCE: Nigerian Journal of Chemical Research (2000), 5, 39-42
CODEN: NJCRBW; ISSN: 1119-0221
PUBLISHER: Nigerian Journal of Chemical Research
DOCUMENT TYPE: Journal
LANGUAGE: English
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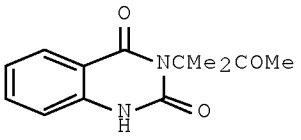
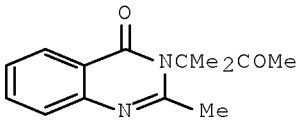


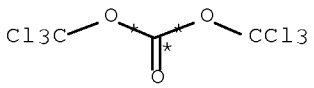
I



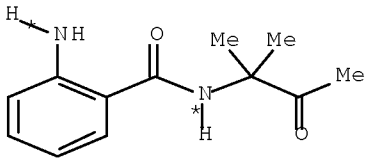
II

AB Ring opening of isatoic anhydride with 1,1-dimethyl-2-propynylamine at 45° in DMF gave 2-H2NC6H4CONHCMe2R (I, R = C.tplbond.CH), while refluxing isatoic anhydride with 1,1-dimethyl-2-propynylamine at 100° in water afforded I (R = COMe). When I (R = C.tplbond.CH) was refluxed in formic acid-water, I (R = COMe) was also obtained, and on cyclization with triphosgene and tri-Et orthoacetate it yielded the quinazolinones II and III, resp.

RX(4) OF 12 ...I + E ===> J

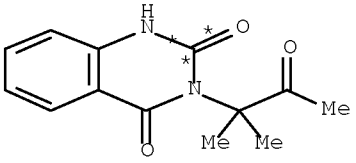


I



E

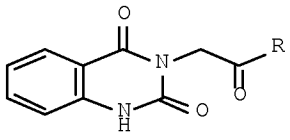
(4) →



J
YIELD 70%

RX(4) RCT I 32315-10-9, E 485322-54-1
RGT K 121-44-8 Et3N
PRO J 485322-55-2
SOL 123-91-1 Dioxane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 6 hours, reflux
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

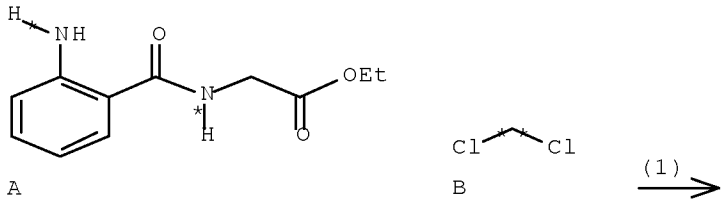
L45 ANSWER 3 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 129:109322 CASREACT Full-text
TITLE: Synthesis of 3-dipeptidyl-2,4(1H,3H)-quinazolinediones as potential anti-hypertensive agents
AUTHOR(S): Rivero, I. A.; Somanathan, R.; Hellberg, L. H.
CORPORATE SOURCE: Centro de Graduados e Investigacion del Instituto Tecnologico de Tijuana, Tijuana, 22000, Mex.
SOURCE: Synthetic Communications (1998), 28(11), 2077-2086
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



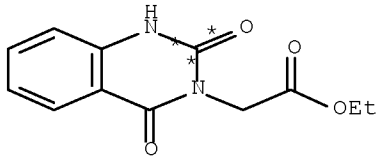
I

AB Quinazolinediones I (R = Trp-OMe, Phe-OEt, Pro-OMe, Gly-OEt, DL-Ala-OMe) bearing a dipeptide moiety have been synthesized as potential anti-hypertensive agents (no data given).

RX(1) OF 9 A + B ===> C...



A B (1)



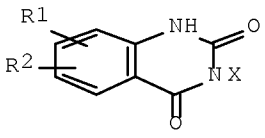
C

RX(1) RCT A 5973-34-2, B 75-09-2
PRO C 58004-83-4
NTE 2 H, 20.deg.
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

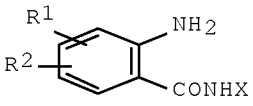
L45 ANSWER 4 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 128:13283 CASREACT Full-text
TITLE: Preparation of dioxoquinazolines
INVENTOR(S): Ueda, Hiroshi; Komatsu, Satoshi; Nishii, Shinji
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09291080	A	19971111	JP 1996-105647	19960425

PRIORITY APPLN. INFO.: JP 1996-105647 19960425
OTHER SOURCE(S): MARPAT 128:13283
GI



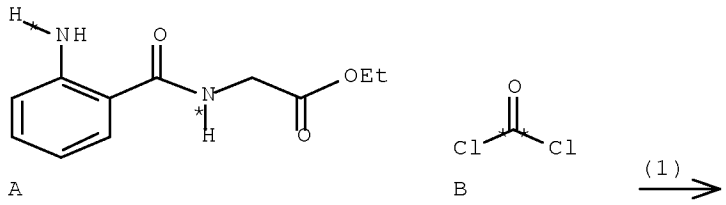
I



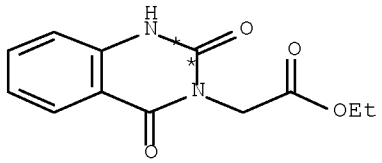
II

AB Title compds. I [R1, R2 = H, halo, NO2, lower (halo)alkyl, (halo)aralkyl, (halo)alkoxy, (halo)alkoxycarbonyl, YNR3R4; R3, R4 = lower alkyl; R3R4 may form ring; Y = bond, lower alkylene, CO; X = lower (halo)alkyl, (halo)aralkyl, ZCO2R5; R5 = lower alkyl, aralkyl; Z = lower alkylene], useful as intermediates for antiinflammatories, drugs for diabetic complications, etc., are prepared by treating anthranilamides II (R1, R2, X = same as I) with COCl2. II (R1 = R2 = H, X = CH2CO2Et) was treated with COCl2 and NEt3 in THF at 5° for 90 min to give 98% I (R1 = R2 = H, X = CH2CO2Et).

RX(1) OF 1 A + B ===> C



A B (1)



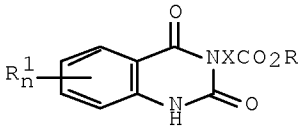
C
YIELD 98%

RX(1) RCT A 5973-34-2, B 75-44-5
RGT D 121-44-8 Et3N
PRO C 58004-83-4
SOL 109-99-9 THF

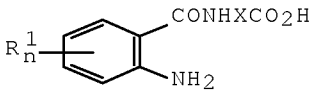
L45 ANSWER 5 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 115:256211 CASREACT Full-text
TITLE: (1,2,3,4-Tetrahydro-2,4-dioxoquinazolin-3-yl)alkanoate esters
INVENTOR(S): Suesse, Manfred; Cleve, Dorothee; Johne, Siegfried
PATENT ASSIGNEE(S): Akademie der Wissenschaften der DDR, Germany
SOURCE: Ger. (East), 4 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 291083	A5	19910620	DD 1989-336570	19891228

PRIORITY APPLN. INFO.: DD 1989-336570 19891228
OTHER SOURCE(S): MARPAT 115:256211
GI



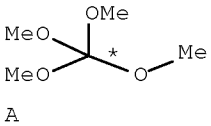
I



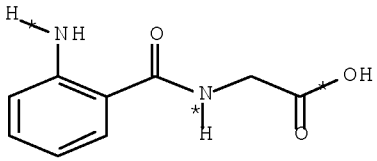
II

AB Title compds. I (R = alkyl; R1 = alkyl, alkoxy, halo, etc.; X = alkylene; n = 0-4) were prepared from amino carboxylic acids II and orthocarbonate esters. Thus, 1.94 g II (X = CH2, n = 0) was refluxed with 4.1 g tetra-Me orthocarbonate for 4 h to give 1.4 g I (R = Me, X = CH2, n = 0).

RX(1) OF 1 A + B ===> C

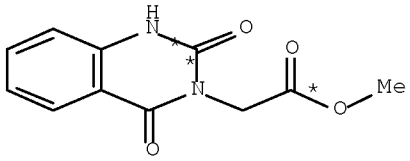


A



B

(1)



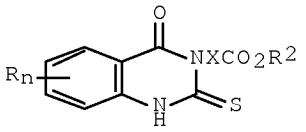
C

RX(1) RCT A 1850-14-2, B 526-21-6
PRO C 82603-69-8

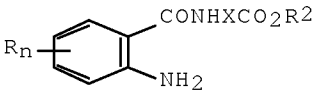
L45 ANSWER 6 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 109:73469 CASREACT Full-text
TITLE: Preparation of (1,2,3,4-tetrahydro-4-oxo-2-thioxoquinazolin-3-yl)-alkanoates as agrochemicals
INVENTOR(S): Suesse, Manfred; Schaks, Angela; Johne, Siegfried
PATENT ASSIGNEE(S): Akademie der Wissenschaften der DDR, Ger. Dem. Rep.
SOURCE: Ger. (East), 5 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 252603	A1	19871223	DD 1986-294469	19860917
PRIORITY APPLN. INFO.:			DD 1986-294469	19860917

GI



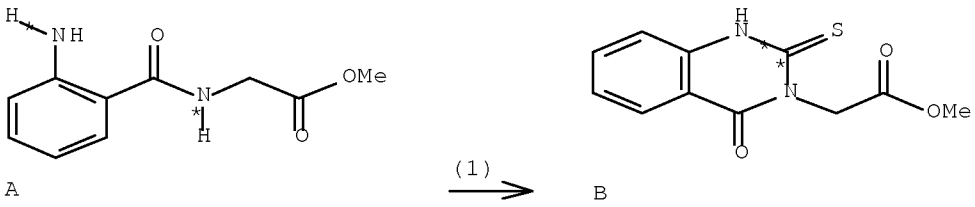
I



II

AB The title compds. [I; R = alkyl, alkoxy, halo, NO2, CN, CF3, alkoxycarbonyl, amino, acyl; R2 = H, alkyl; X = (substituted) C1-10 alkylene; n = 0-4] useful as agrochems., for example as fungicides (no data), were prepared by cyclocondensation of (aminobenzoyl)amino acids II with CSCl2 in H2O or an organic solvent in the presence of a base, optionally followed by hydrolysis. o-Aminohippuric acid Me ester and Et3N in CHCl3 at 5° were treated with CSCl2 in CHCl3. The mixture was then stirred 2 h at room temperature and 30 min at 35° to give 44% I (n = 0, R2 = Me, X = CH2).

RX(1) OF 3 A ===> B...



A B

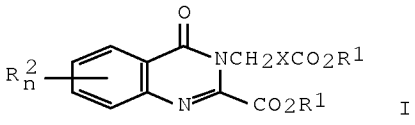
RX(1) RCT A 82185-40-8
PRO B 85716-94-5

L45 ANSWER 7 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 108:131849 CASREACT Full-text
TITLE: Preparation of 2-alkoxycarbonyl-3,4-dihydro-4-oxoquinazolin-3-yl-alkanoates as agrochemical fungicides
INVENTOR(S): Suesse, Manfred; Ermisch, Christine; Johne, Siegfried
PATENT ASSIGNEE(S): Akademie der Wissenschaften der DDR, Ger. Dem. Rep.
SOURCE: Ger. (East), 4 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 247450	A1	19870708	DD 1986-288515	19860331

PRIORITY APPLN. INFO.: DD 1986-288515 19860331

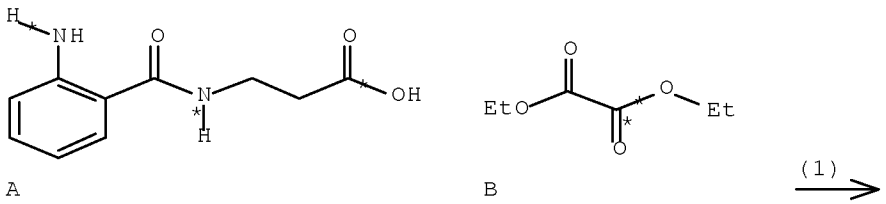
GI



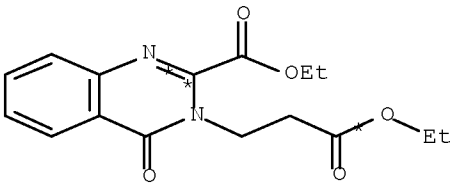
I

AB The title compds. (I; R1 = alkyl; R2 = alkyl, alkoxy, halo, CN, NO2, CF3; n = 0-4) were prepared as agrochem. fungicides (no data). A mixture of 3-(o-aminobenzoylamino)propanoic acid and excess di-Et oxalate was heated at 140° for 4 h to give 25% I (R1 = Et, X = CH2, 1 = 0).

RX(1) OF 1 A + B ===> C



A B (1)



C

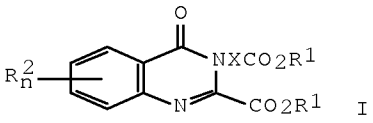
RX(1) RCT A 13135-92-7, B 95-92-1
PRO C 107466-56-8

L45 ANSWER 8 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 108:94592 CASREACT Full-text
TITLE: Preparation of 2-(alkoxycarbonyl)-4-oxo-3-quinazolinealkaroates as agrochemical fungicides

INVENTOR(S): Suesse, Manfred; Ermisch, Christine; Johne, Siegfried
PATENT ASSIGNEE(S): Akademie der Wissenschaften der DDR, Ger. Dem. Rep.
SOURCE: Ger. (East), 4 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 247449	A1	19870708	DD 1986-288514	19860331

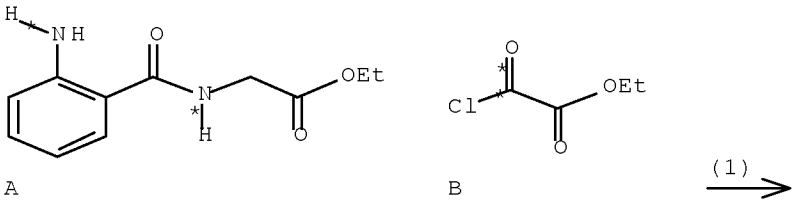
PRIORITY APPLN. INFO.: DD 1986-288514 19860331
GI



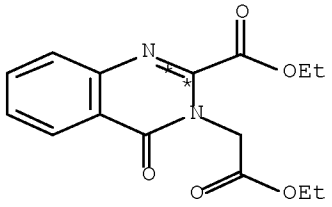
I

AB The title compds. (I; R1 = alkyl; R2 = alkyl, alkoxy, halo, CN, NO2, CF3; X = C1-10 alkylene; n = 0-4) were prepared as agrochem. fungicides (no data). To a 10° solution of Et 2-amino-hippurate in MeCN were added Et3N and ClCOCO2Et. The temperature was gradually raised to 80° over 1 h and the mixture was stirred for another 30 min to give 10% I (R1 = Et, X = CH2, n = 0).

RX(1) OF 1 A + B ===> C



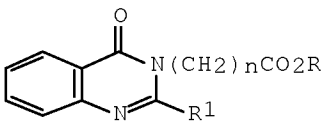
A B (1)



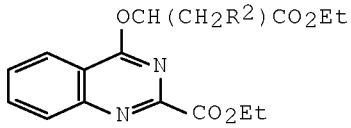
C

RX(1) RCT A 5973-34-2, B 4755-77-5
PRO C 64697-12-7

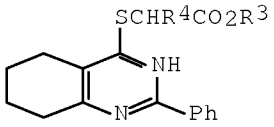
L45 ANSWER 9 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 106:138387 CASREACT Full-text
TITLE: Quinazolinecarboxylic acid. Synthesis of alkyl[2-(ethoxycarbonyl)-3,4-dihydro-4-oxoquinazolin-3-yl]-, [2-(ethoxycarbonyl)quinazolin-4-yloxy]- and (5,6,7,8-tetrahydro-2-phenylquinazolin-4-ylthio)alkanoates
AUTHOR(S): Suesse, Manfred; Adler, Frank; Johne, Siegfried
CORPORATE SOURCE: Inst. Biochem. Pflanzen Halle, Dtsch. Akad. Wiss., Halle/Saale, DDR-4010, Ger. Dem. Rep.
SOURCE: Helvetica Chimica Acta (1986), 69(5), 1017-24
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



II



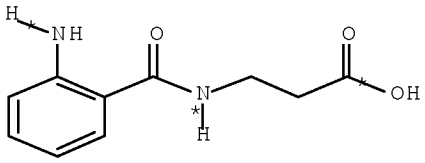
IV



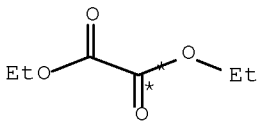
V

AB Cyclization of 2-H2NC6H4CONH(CH2)nCO2Et (I, n = 2, 3) with EtO2CCO2Et gave quinazolines II (R = Et, R1 = CO2Et), whereas, condensation of I (n = 1) with ClCOCO2Et gave a mixture of 2-EtO2CCONHC6H4CONHCH2CO2Et and II (n = 1, R = Et, R1 = CO2Et). Cyclization of 2-H2NC6H4CONH2 (III) with EtO2CCO2Et followed by condensation with BrCH2CO2R (R = Me, Et) gave II (n = 1, R = Me, Et, R1 = CO2Et), whereas, cyclization of III with EtO2CCO2Et followed by condensation with R2CH2CHBrCO2Et (R2 = H, Me) gave quinazoline esters IV. Condensation of III with ClCOCH2CH2CO2Me gave 2- H2NCOC6H4NHCOCH2CH2CO2Me which was cyclized with BrCH2CO2Et to give II (n = 1, R = Et, R1 = CH2CH2CO2CH2CO2Et). Quinazoline thioethers V (R3 = Me, Et, R4 = H, Et, CHMe2) were prepared by aminolysis of 5,6,7,8-tetrahydro-1,3- benzoxazine-4(3H)-thione followed by condensation with BrCHR4CO2R3.

RX(1) OF 27 A + B ===> C

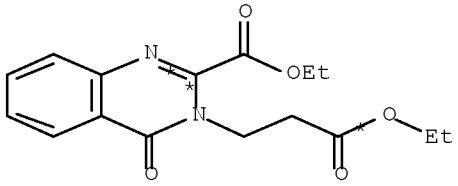


A



B

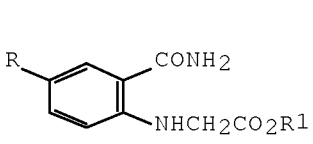
(1)



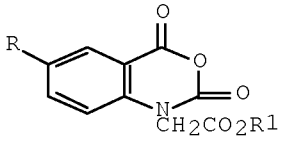
C
YIELD 25%

RX(1) RCT A 13135-92-7, B 95-92-1
PRO C 107466-56-8

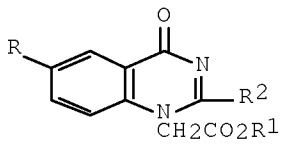
L45 ANSWER 10 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 106:102208 CASREACT Full-text
TITLE: Quinazolinecarboxylic acids. 5. Synthesis of 1,4-dihydroquinazolin-4-on-1-ylacetic acids and esters
AUTHOR(S): Suesse, Manfred; Johne, Siegfried
CORPORATE SOURCE: Inst. Biochem. Pflanzen, Dtsch. Akad. Wiss., Halle, DDR-4020, Ger. Dem. Rep.
SOURCE: Monatshefte fuer Chemie (1986), 117(4), 499-509
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I



II

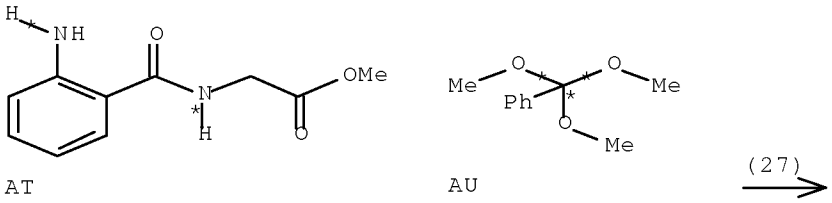


III

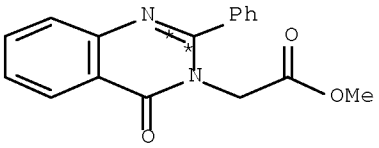
IV

AB Cyclization of aminobenzamides I (R = H, Cl, Br; R1 = Me, Et), prepared by reaction of benzoxaziniediones II with NH3, with HC(OEt)3 gave esters III (R2 = H), hydrolysis of III lead to the title acids III (R1 = H). 2-Substituted quinazolinones III (R2 = Me, Et, Ph, 4-O2NC6H4, 4-HOC6H4, 2-ClC6H4) could be obtained by reaction of I with acid chlorides or by reaction of II with amidines. Quinazolinone IV was synthesized in a similar way. The amide 2-H2NC6H4CONHCH2CO2Me showed reaction behavior different from that of I.

RX(27) OF 48 AT + AU ===> AV



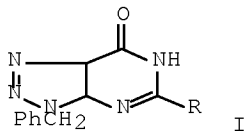
AT AU



AV
YIELD 36%

RX(27) RCT AT 82185-40-8, AU 707-07-3
PRO AV 106634-20-2

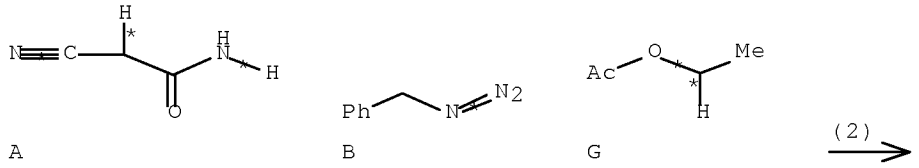
L45 ANSWER 11 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 105:208821 CASREACT Full-text
TITLE: A facile one pot synthesis of 2,9-disubstituted 8-azapurin-6-ones (3,5-disubstituted 7-hydroxy-3H-1,2,3-triazolo[4,5-d]pyrimidines)
AUTHOR(S): Barili, Pier Luigi; Biagi, Giuliana; Livi, Oreste; Scartoni, Valerio
CORPORATE SOURCE: Ist. Chim. Org., Univ. Pisa, Pisa, 56100, Italy
SOURCE: Journal of Heterocyclic Chemistry (1985), 22(6), 1607-9
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



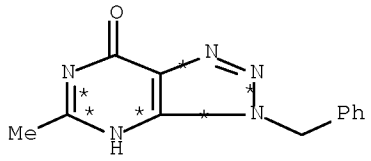
I

AB Cyclization of NCCH2CONH2, PhCH2N3, and RCO2R1 [R = H, Me, Et, Pr, MeOCH2CH2, CH(OEt)2, CH2CH2CO2H, CO2Et, Ph, PhCH2, BzNHCH2; R1 = Me, Et] gave 43-95% title compds. I.

RX(2) OF 11 A + B + G ===> H



A B G (2)



H

RX(2) RCT A 107-91-5, B 622-79-7

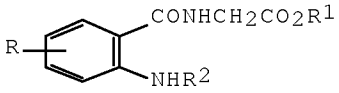
STAGE(1)
RGT E 141-52-6 NaOEt
SOL 64-17-5 EtOH

STAGE(2)
RCT G 141-78-6
SOL 64-17-5 EtOH

PRO H 71492-05-2

L45 ANSWER 12 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 106:32964 CASREACT Full-text
TITLE: Quinazolincarboxylic acids. IX. Synthesis and reactions of 2-ureidohippuric acids and their esters
AUTHOR(S): Suesse, Manfred; Johne, Siegfried
CORPORATE SOURCE: Inst. Biochem. Pflanzen Halle, Dtsch. Akad. Wiss., Halle/Saale, DDR-4020/3, Ger. Dem. Rep.

SOURCE: Zeitschrift fuer Chemie (1985), 25(11), 403-4
CODEN: ZECEAL; ISSN: 0044-2402
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



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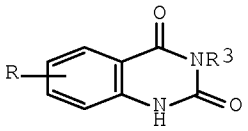
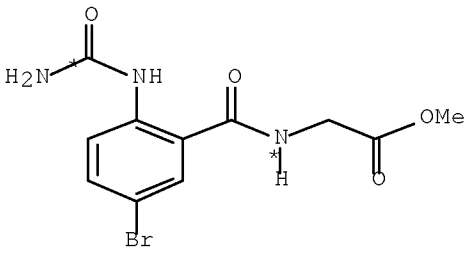


II

AB The aminohippuric acids I (R = H, 5-Br, 3,5-Br2, 3,5-Cl2; R1 = H, Me; R2 = H) were treated with KCNO to give the ureido derivs. I (R2 = CONH2). I (R = 5-Br, R1 = Me, R2 = CONH2) was heated at 200-210° under N to give the quinazoline II (R3 = CH2CO2Me). I (R = H, R1 = Me, R2 = CONH2) was treated with KOH in EtOH to give II (R3 = H).

RX(7) OF 12 ...H ===> O



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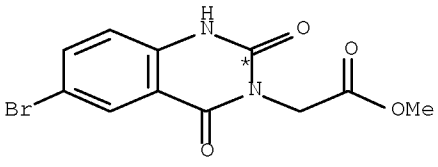
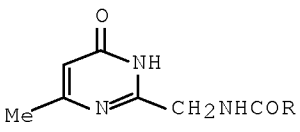
(7)



O

RX(7) RCT H 105217-21-8
PRO O 106047-54-5
SOL 7727-37-9 N2

L45 ANSWER 13 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 96:85497 CASREACT Full-text
TITLE: 2-[(Acylamino)methyl]-6-methylpyrimidin-4(3H)-ones. Novel precursors for the synthesis of imidazo[1,5-a]pyrimidines and imidazo[4,5-b]pyridines
AUTHOR(S): Katagiri, Nobuya; Koshihara, Akemi; Atsuumi, Shugo; Kato, Tetsuzo
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SOURCE: Journal of Organic Chemistry (1982), 47(1), 167-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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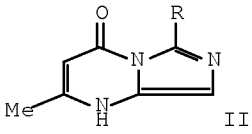

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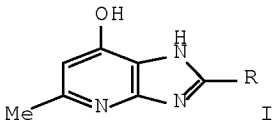
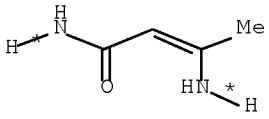
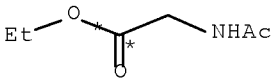


III

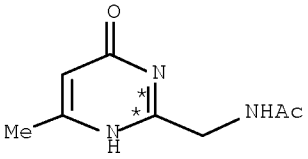
AB Pyrimidinones I (R = Me, CHMe2, Ph), prepared from 3-aminocrotonamide and Et N-acylglycinates, are novel and versatile precursors for the preparation of imidazopyrimidines II (R = Me, CHMe2) and imidazopyridines III (R = Me, CHMe2, Ph).

RX(3) OF 30 F + G ===> H...



F


G
(3)



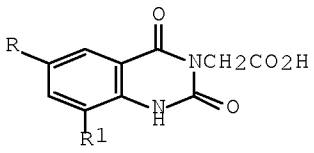
H
YIELD 71%

RX(3) RCT F 15846-25-0, G 1906-82-7
PRO H 79898-99-0

L45 ANSWER 14 OF 18 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 96:162734 CASREACT Full-text
TITLE: Quinazoline-2,4-dione-3-acetic acids
INVENTOR(S): Suesse, Manfred; Johne, Siegfried
PATENT ASSIGNEE(S): Akademie der Wissenschaften der DDR, Ger. Dem. Rep.
SOURCE: Ger. (East), 16 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 151308	A1	19811014	DD 1980-221623	19800606

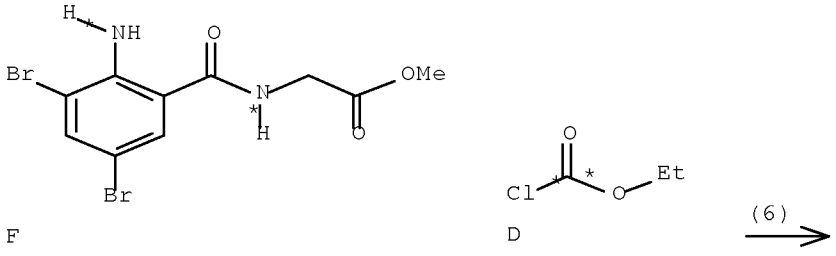
PRIORITY APPLN. INFO.: DD 1980-221623 19800606
GI



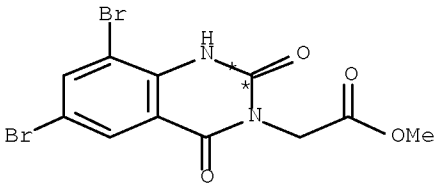
I

AB Quinazolinediones I (R, R1 = H, halogen, NO2, alkyl, alkoxy, CO2H) were prepared Thus 6,8-dibromoisatoic anhydride was treated with H2NCH2CO2Me.HCl to give 90% 2,3,5-H2N(Br)2C6H2CONHCH2CO2Me which was cyclized with ClCO2Et and saponified to give 50% I (R = R1 = Br).

RX(6) OF 13 ...F + D ===> H



F D (6)



H

RX(6) RCT F 81438-16-6, D 541-41-3
PRO H 81438-17-7

L45 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:591360 CAPLUS Full-text
DOCUMENT NUMBER: 147:31135
TITLE: Pyrimidinone derivatives as calcilytic compounds and their preparation, pharmaceutical compositions and use as calcium receptor inhibitors for treatment of bone and mineral diseases
INVENTOR(S): Ku, Thomas Wen Fu; Lin, Hong; Luengo, Juan I.; Marquis, Robert W., Jr.; Ramanjulu, Joshi M.; Trout, Robert; Yamashita, Dennis S.
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 251pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007062370	A2	20070531	WO 2006-US61150	20061121
WO 2007062370	A3	20071122		

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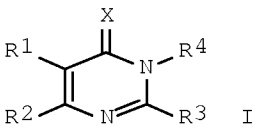
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-738731P P 20051122
US 2005-739067P P 20051122
OTHER SOURCE(S): MARPAT 147:31135
GI



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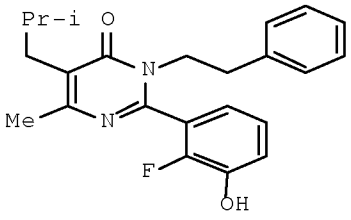


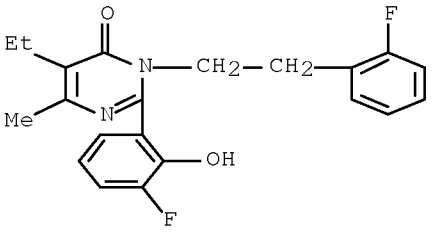
II

AB Novel calcilytic compds. of formula I, pharmaceutical compns., methods of synthesis and methods of using them are provided. Compds. of formula I wherein C is O and S; R1 and R2 are independently H, halo, CN, C1-10 alkyl, C2-6 alkenyl, cycloalkyl, (hetero)aryl, etc.; R3 is (un)substituted (hetero)aryl; R4 is (un)substituted (hetero)aryl, (un)substituted heterocyclyl, (un)substituted cycloalkyl-C1-4 alkyl, etc.; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by alkylation of Et 3-oxobutanoate with 3-bromo-2-methyl-1-propene; the resulting Et 2-acetyl-4-methyl-4-pentenoate underwent amidation with phenethylamine to give 2-acetyl-4-methyl-N-(phenethyl)-4- pentenamide, which underwent hydrogenation to give 2-acetyl-4-methyl-N- (phenethyl)-4-pentanamide, which underwent cyclization with 2-fluoro-3-methoxybenzamide to give 2-[2-fluoro-3-methoxyphenyl]-6-methoxy- 5-(2-methylpropyl)-3-(2-phenylethyl)-4(3H)-pyrimidinone, which underwent demethylation to give compound II. All the invention compds. were evaluated for their calcium receptor inhibitory activity.

IT 938179-15-8P 938179-98-7P 938180-14-4P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

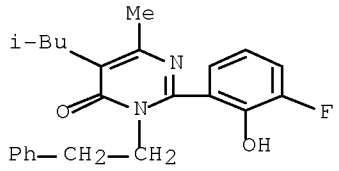
RN 938179-15-8 CAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)

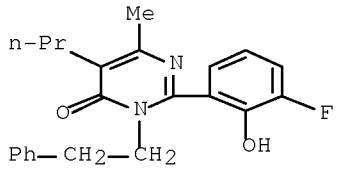


RN 938179-98-7 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938180-14-4 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-propyl- (CA INDEX NAME)



IT 780771-55-3P 938177-03-8P 938177-43-6P
938177-48-1P 938177-52-7P 938177-71-0P
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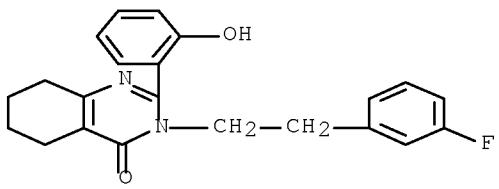
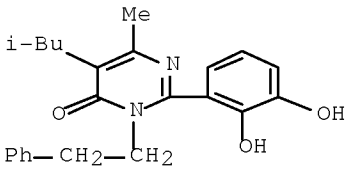
938179-49-8P 938179-50-1P 938179-51-2P
938179-54-5P 938179-99-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

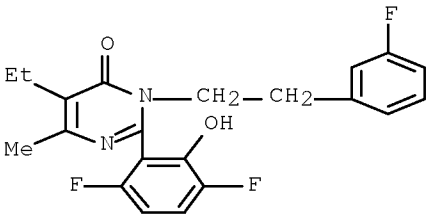
RN 780771-55-3 CAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)- (CA INDEX NAME)



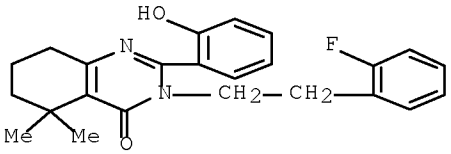
RN 938177-03-8 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(2,3-dihydroxyphenyl)-6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



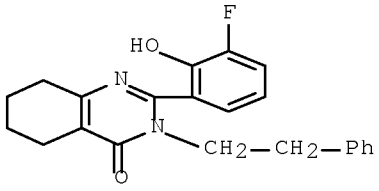
RN 938177-43-6 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3,6-difluoro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



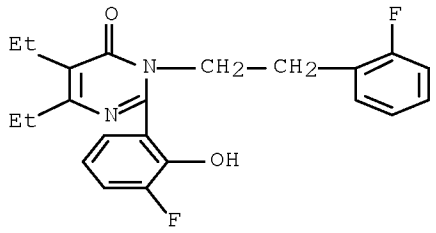
RN 938177-48-1 CAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(2-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-5,5-dimethyl- (CA INDEX NAME)



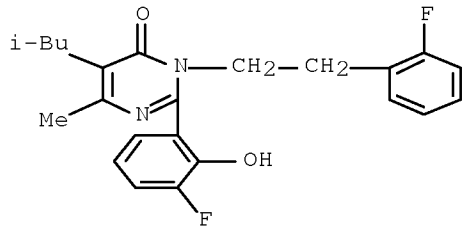
RN 938177-52-7 CAPLUS
CN 4(3H)-Quinazolinone, 2-(3-fluoro-2-hydroxyphenyl)-5,6,7,8-tetrahydro-3-(2-phenylethyl)- (CA INDEX NAME)



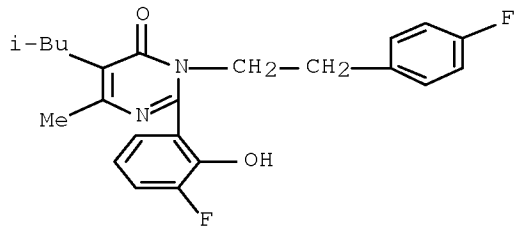
RN 938177-71-0 CAPLUS
CN 4(3H)-Pyrimidinone, 5,6-diethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]- (CA INDEX NAME)



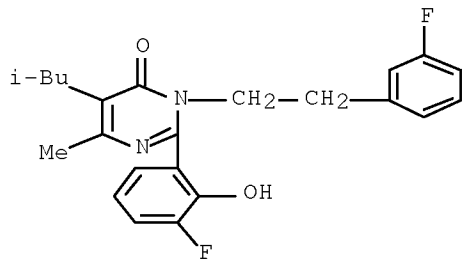
RN 938177-76-5 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-methyl-5-(2-methylpropyl)- (CA INDEX NAME)



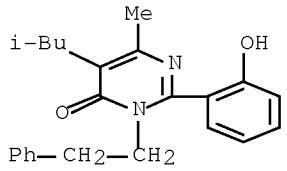
RN 938177-80-1 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(4-fluorophenyl)ethyl]-6-methyl-5-(2-methylpropyl)- (CA INDEX NAME)



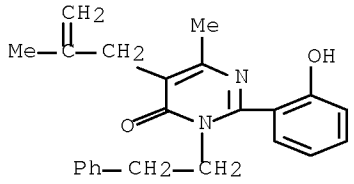
RN 938177-82-3 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(2-methylpropyl)- (CA INDEX NAME)



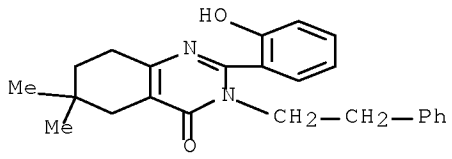
RN 938178-59-7 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



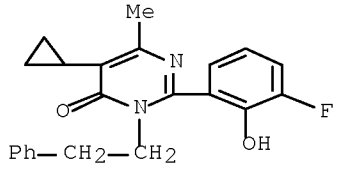
RN 938178-60-0 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(2-methyl-2-propen-1-yl)-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938178-63-3 CAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-6,6-dimethyl-3-(2-phenylethyl)- (CA INDEX NAME)

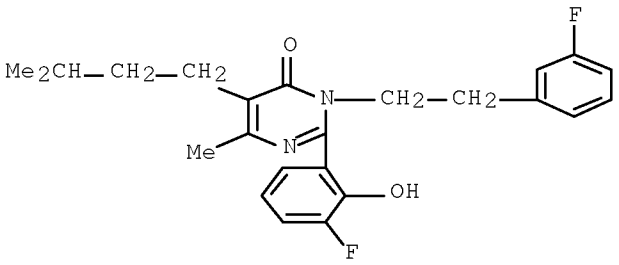


RN 938178-65-5 CAPLUS
CN 4(3H)-Pyrimidinone, 5-cyclopropyl-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)

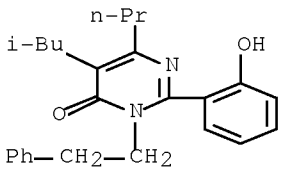


RN 938178-66-6 CAPLUS

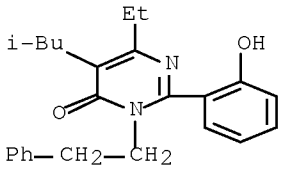
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(3-methylbutyl)- (CA INDEX NAME)



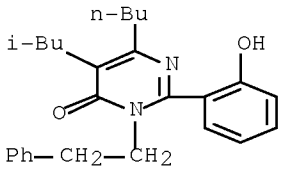
RN 938178-79-1 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5-(2-methylpropyl)-3-(2-phenylethyl)-6-propyl- (CA INDEX NAME)



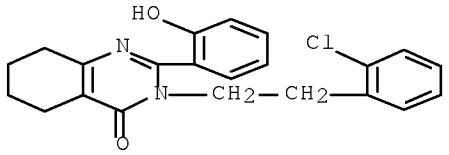
RN 938178-80-4 CAPLUS
CN 4(3H)-Pyrimidinone, 6-ethyl-2-(2-hydroxyphenyl)-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



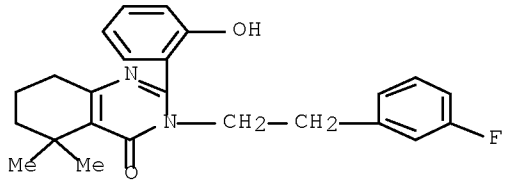
RN 938178-81-5 CAPLUS
CN 4(3H)-Pyrimidinone, 6-butyl-2-(2-hydroxyphenyl)-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



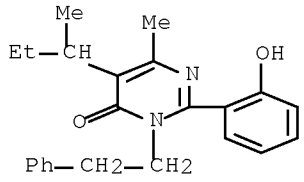
RN 938178-90-6 CAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(2-chlorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)- (CA INDEX NAME)



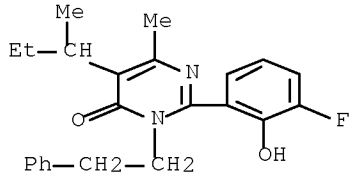
RN 938178-91-7 CAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-5,5-dimethyl- (CA INDEX NAME)



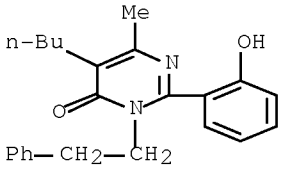
RN 938178-98-4 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(1-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



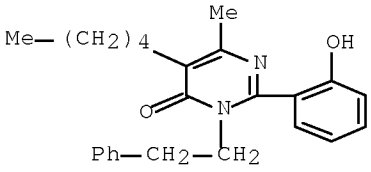
RN 938178-99-5 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(1-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



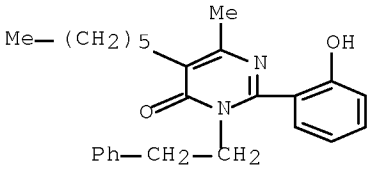
RN 938179-00-1 CAPLUS
CN 4(3H)-Pyrimidinone, 5-butyl-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



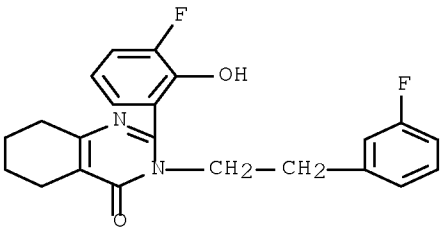
RN 938179-01-2 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-pentyl-3-(2-phenylethyl)- (CA INDEX NAME)



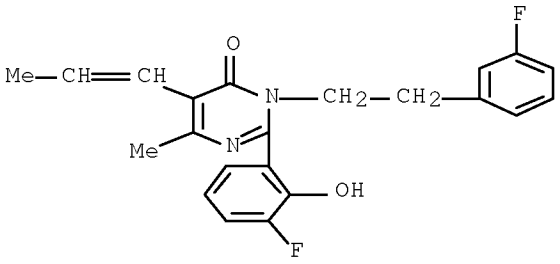
RN 938179-02-3 CAPLUS
CN 4(3H)-Pyrimidinone, 5-hexyl-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



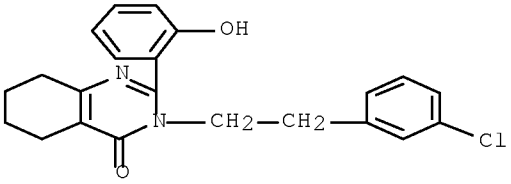
RN 938179-08-9 CAPLUS
CN 4(3H)-Quinazolinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro- (CA INDEX NAME)



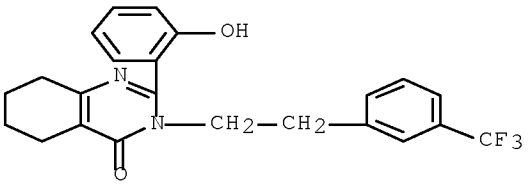
RN 938179-16-9 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(1-propen-1-yl)- (CA INDEX NAME)



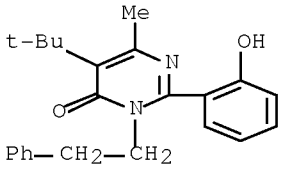
RN 938179-21-6 CAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-chlorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)- (CA INDEX NAME)



RN 938179-23-8 CAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-3-[2-[3-(trifluoromethyl)phenyl]ethyl]- (CA INDEX NAME)

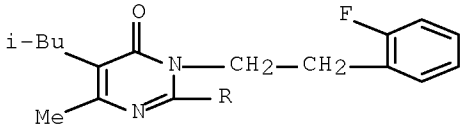


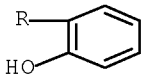
RN 938179-33-0 CAPLUS
CN 4(3H)-Pyrimidinone, 5-(1,1-dimethylethyl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



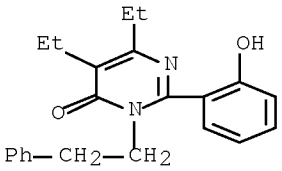
RN 938179-42-1 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-

methyl-5-(2-methylpropyl)- (CA INDEX NAME)

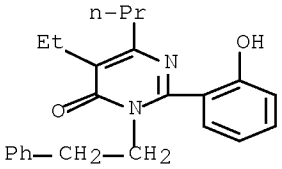




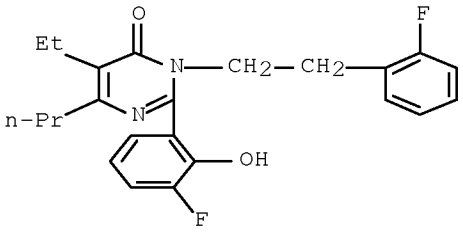
RN 938179-44-3 CAPLUS
CN 4(3H)-Pyrimidinone, 5,6-diethyl-2-(2-hydroxyphenyl)-3-(2-phenylethyl)-
(CA INDEX NAME)



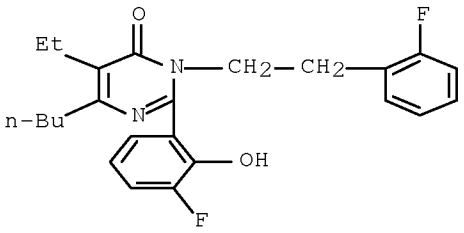
RN 938179-45-4 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-hydroxyphenyl)-3-(2-phenylethyl)-6-propyl-
(CA INDEX NAME)



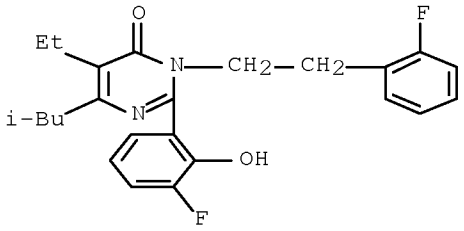
RN 938179-47-6 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-
fluorophenyl)ethyl]-6-propyl- (CA INDEX NAME)



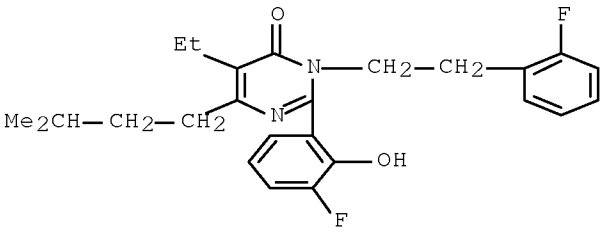
RN 938179-49-8 CAPLUS
CN 4(3H)-Pyrimidinone, 6-butyl-5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]- (CA INDEX NAME)



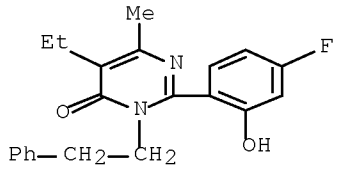
RN 938179-50-1 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-(2-methylpropyl)- (CA INDEX NAME)



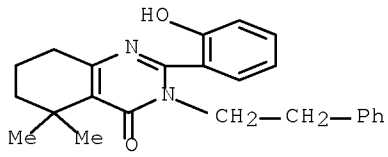
RN 938179-51-2 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-(3-methylbutyl)- (CA INDEX NAME)



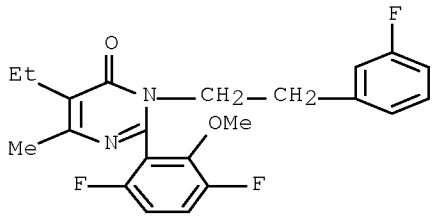
RN 938179-54-5 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(4-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



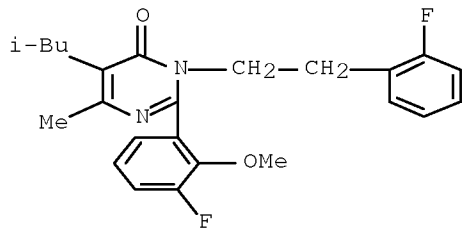
RN 938179-99-8 CAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-5,5-dimethyl-3-(2-phenylethyl)- (CA INDEX NAME)



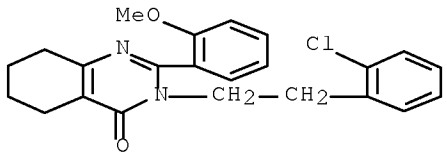
IT 938180-43-9P 938180-58-6P 938181-03-4P
938181-16-9P 938181-18-1P 938181-44-3P
938181-72-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)
RN 938180-43-9 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3,6-difluoro-2-methoxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



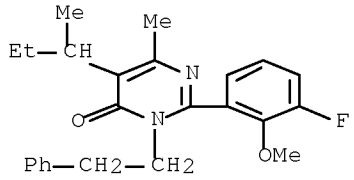
RN 938180-58-6 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-methoxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-methyl-5-(2-methylpropyl)- (CA INDEX NAME)



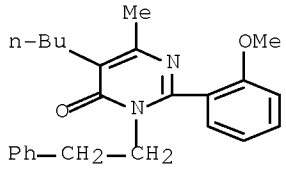
RN 938181-03-4 CAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(2-chlorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-methoxyphenyl)- (CA INDEX NAME)



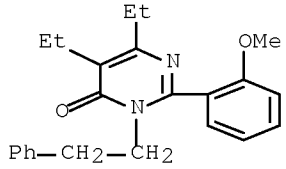
RN 938181-16-9 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-methoxyphenyl)-6-methyl-5-(1-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938181-18-1 CAPLUS
CN 4(3H)-Pyrimidinone, 5-butyl-2-(2-methoxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)

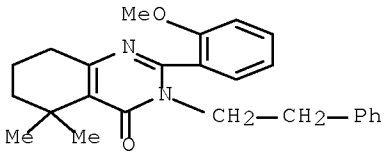


RN 938181-44-3 CAPLUS
CN 4(3H)-Pyrimidinone, 5,6-diethyl-2-(2-methoxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938181-72-7 CAPLUS

CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-methoxyphenyl)-5,5-dimethyl-3-(2-phenylethyl)- (CA INDEX NAME)



L45 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:605352 CAPLUS Full-text
DOCUMENT NUMBER: 145:83371
TITLE: Preparation of prodrug constructs of pyrimidinone compounds as calcilytics
INVENTOR(S): Shcherbakova, Irina; Wermuth, Camille G.; Jeannot, Frederic; Ciapetti, Paola; Roques, Virginie; Jung, Laetitia M.; Balandrin, Manuel F.; Nair, Satheesh, K.; Swierczek, Krzysztof; McCaffrey, Jennifer; Heaton, William L.; Breinholt, Jeff A.; Conklin, Rebecca L.
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006066070	A2	20060622	WO 2005-US45565	20051216
WO 2006066070	A3	20060921		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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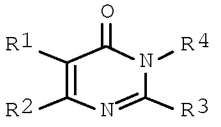
PRIORITY APPLN. INFO.: US 2004-637115P P 20041217
OTHER SOURCE(S): MARPAT 145:83371
GI



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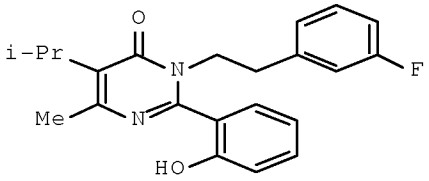
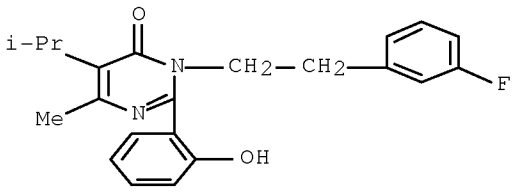


II

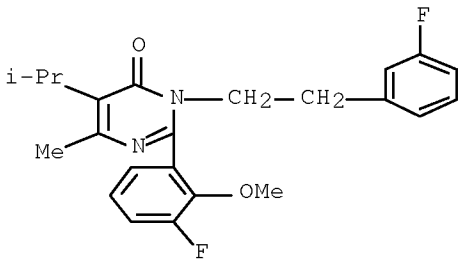
AB Calcilytic pyrimidinones I [R1 and R2 = H, halo, CN, CF3, etc.; R3 = (un)substituted aryl group; R4 = H, alkyl, aryl, etc.], and prodrugs as well as pharmaceutically acceptable salts thereof, are prepared for use in treating disease or disorders characterized by abnormal bone or mineral homeostasis. Thus, e.g., II was prepared by amidation of anisoyl chloride with 2-amino-2-isopropylbut-2-enoic acid Me ester (preparation given) followed by cyclization with 3-fluorphenethyl amine and demethylation. Calcilytic compds. are compds. capable of inhibiting calcium receptor activity. Assays for determining calcium receptor inhibition are described with parameter of desirable IC50 values given. Methods for preparing these compds., oral bioavailability of these compds., pharmaceutical compns. containing these compds. and their use as calcium receptor antagonists are also disclosed.

IT 780771-48-4P 893053-18-4P 893053-34-4P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)

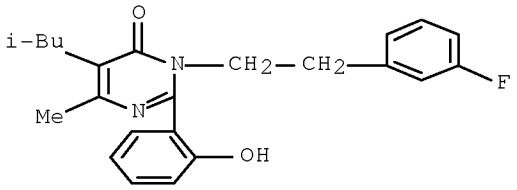
RN 780771-48-4 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



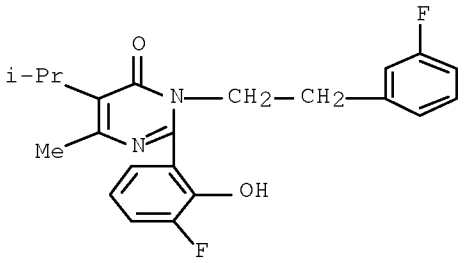
RN 893053-18-4 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-methoxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



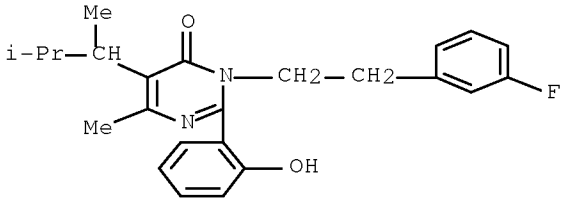
RN 893053-34-4 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(2-methylpropyl)- (CA INDEX NAME)



IT 893053-26-4P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)
RN 893053-26-4 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



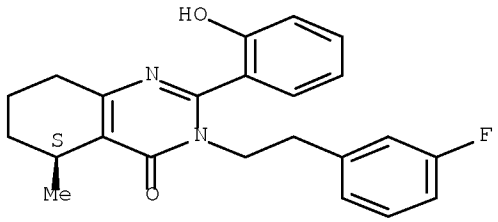
IT 893054-83-6P 893054-99-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)
RN 893054-83-6 CAPLUS
CN 4(3H)-Pyrimidinone, 5-(1,2-dimethylpropyl)-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



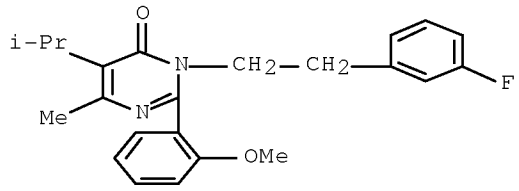
RN 893054-99-4 CAPLUS

CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-5-methyl-, (5S)- (CA INDEX NAME)

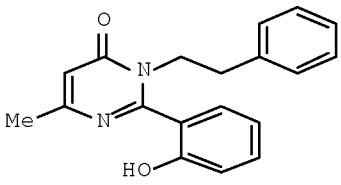
Absolute stereochemistry.



IT 780771-51-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)
RN 780771-51-9 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-methoxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



L45 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:378882 CAPLUS Full-text
DOCUMENT NUMBER: 143:59927
TITLE: Design, new synthesis, and calcilytic activity of substituted 3H-pyrimidin-4-ones
AUTHOR(S): Shcherbakova, Irina; Huang, Guangfei; Geoffroy, Otto J.; Nair, Satheesh K.; Swierczek, Krzysztof; Balandrin, Manuel F.; Fox, John; Heaton, William L.; Conklin, Rebecca L.
CORPORATE SOURCE: Drug Discovery, NPS Pharmaceuticals, Inc., Salt Lake City, UT, 84108, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(10), 2537-2540
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:59927
GI

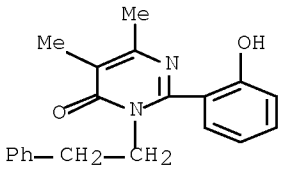


I

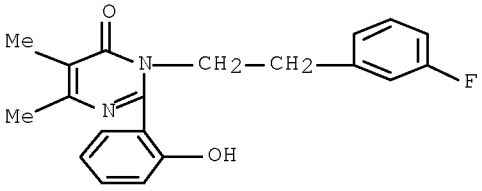
AB Design, synthesis, structure-activity relationship studies and calcium receptor antagonist (calcilytic) properties of 3H-pyrimidin-4-ones, e.g., I, are described. The pyrimidinones were synthesized by multistep procedures.

IT 780771-35-9P 780771-41-7P 780771-43-9P
780771-44-0P 780771-47-3P 780771-48-4P
780771-53-1P 780771-54-2P 780771-55-3P
780771-56-4P 780771-57-5P 780771-58-6P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

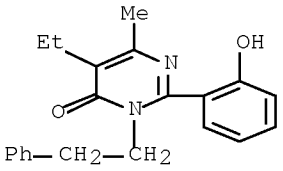
RN 780771-35-9 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5,6-dimethyl-3-(2-phenylethyl)- (CA INDEX NAME)



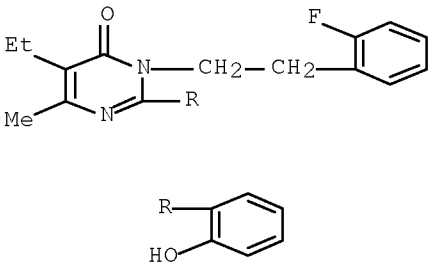
RN 780771-41-7 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl- (CA INDEX NAME)



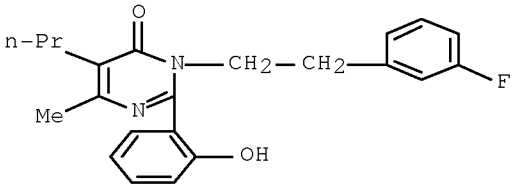
RN 780771-43-9 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



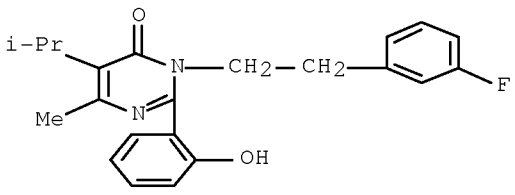
RN 780771-44-0 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



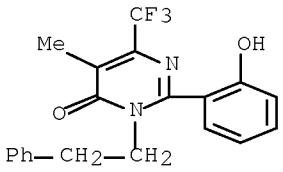
RN 780771-47-3 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-propyl- (CA INDEX NAME)



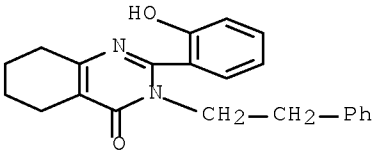
RN 780771-48-4 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



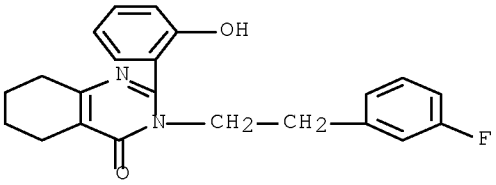
RN 780771-53-1 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5-methyl-3-(2-phenylethyl)-6-(trifluoromethyl)- (CA INDEX NAME)



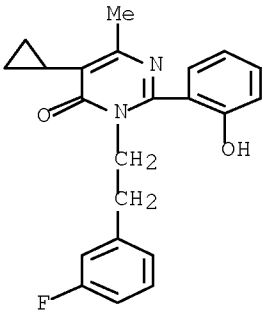
RN 780771-54-2 CAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



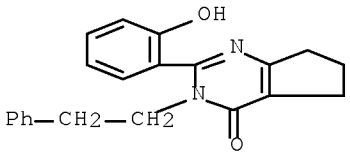
RN 780771-55-3 CAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)- (CA INDEX NAME)



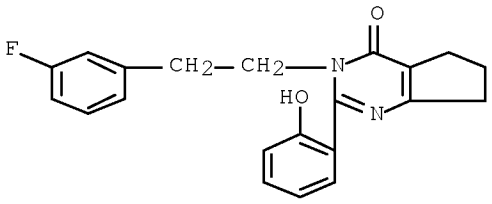
RN 780771-56-4 CAPLUS
CN 4(3H)-Pyrimidinone, 5-cyclopropyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



RN 780771-57-5 CAPLUS
CN 4H-Cyclopentapyrimidin-4-one, 3,5,6,7-tetrahydro-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (9CI) (CA INDEX NAME)



RN 780771-58-6 CAPLUS
CN 4H-Cyclopentapyrimidin-4-one, 3-[2-(3-fluorophenyl)ethyl]-3,5,6,7-tetrahydro-2-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:902338 CAPLUS Full-text
DOCUMENT NUMBER: 141:366249
TITLE: Preparation of pyrimidinone compounds as calcilytics
INVENTOR(S): Shcherbakova, Irina V.; Balandrin, Manuel F.; Huang, Guangfei; Geoffroy, Otto; Fox, John; Marquis, Robert; Yamashita, Dennis Shinji; Luengo, Juan; Wang, Wenyong
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA; Glaxosmithkline
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092120	A2	20041028	WO 2004-US10638	20040407
WO 2004092120	A3	20050414		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004230903	A1	20041028	AU 2004-230903	20040407

CA 2521129	A1	20041028	CA 2004-2521129		20040407
EP 1615897	A2	20060118	EP 2004-749814		20040407
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR					
CN 1835928	A	20060920	CN 2004-80009255		20040407
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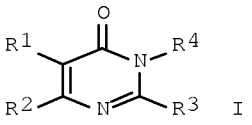
US 2007197555	A1	20070823	US 2006-552363		20061120
PRIORITY APPLN. INFO.:			US 2003-460859P	P	20030407
			US 2003-479323P	P	20030618
			WO 2004-US10638	W	20040407

OTHER SOURCE(S): CASREACT 141:366249; MARPAT 141:366249

GI



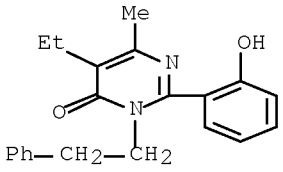
I

AB Title compds. I [R1-2 = H, halo, CN, CF3, etc.; R3 = aryl; R4 = H, alkyl, etc.] are prepared For instance, 2-(2-Hydroxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one is prepared from o-hydroxybenzonitrile, acetyl chloride and Me acetoacetate. Compds. of the invention have IC50 values < 30 μM in a calcium receptor inhibition assay. I are useful for the treatment of abnormal bone or mineral homeostasis.

IT 780771-43-9P, 5-Ethyl-2-(2-hydroxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one 780771-51-9P, 3-[2-(3-Fluorophenyl)ethyl]-5-isopropyl-2-(2-methoxyphenyl)-6-methyl-3H-pyrimidin-4-one
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrimidinone compds. as calcilytics)

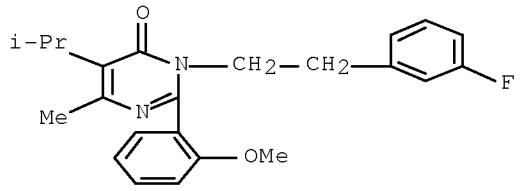
RN 780771-43-9 CAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



RN 780771-51-9 CAPLUS

CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-methoxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)

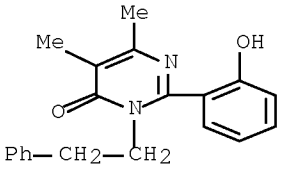


IT 780771-35-9P, 2-(2-Hydroxyphenyl)-5,6-dimethyl-3-phenethyl-3H-pyrimidin-4-one 780771-40-6P, 3-[2-(2-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl-3H-pyrimidin-4-one 780771-41-7P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl-3H-pyrimidin-4-one 780771-42-8P, 3-[2-(4-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl-3H-pyrimidin-4-one 780771-44-0P, 5-Ethyl-3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-45-1P 780771-46-2P, 5-Ethyl-3-[2-(4-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-47-3P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-propyl-3H-pyrimidin-4-one 780771-48-4P , 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5-isopropyl-6-methyl-3H-pyrimidin-4-one 780771-52-0P, 3-[2-(2-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5-isopropyl-6-methyl-3H-pyrimidin-4-one 780771-53-1P, 2-(2-Hydroxyphenyl)-5-methyl-3-phenethyl-6-trifluoromethyl-3H-pyrimidin-4-one 780771-54-2P, 2-(2-Hydroxyphenyl)-3-phenethyl-5,6,7,8-tetrahydro-3H-quinazolin-4-one 780771-55-3P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6,7,8-tetrahydro-3H-quinazolin-4-one 780771-56-4P, 5-Cyclopropyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-57-5P, 2-(2-Hydroxyphenyl)-3-phenethyl-3,5,6,7-tetrahydrocyclopenta[1,2-d]pyrimidin-4-one 780771-58-6P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-3,5,6,7-tetrahydrocyclopenta[1,2-d]pyrimidin-4-one 780771-59-7P, 5-Ethyl-2-(2-methoxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one 780771-62-2P, 5-Ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-64-4P, 5-Ethyl-2-(5-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-65-5P, 5-Ethyl-2-(2-fluoro-6-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-67-7P, 2-(5-Chloro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-68-8P, 2-(5-Bromo-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-69-9P, 5-Ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-3-isopropylphenyl)-6-methyl-3H-pyrimidin-4-one 780771-71-3P, 2-(3,5-Dibromo-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-72-4P, 5-Ethyl-2-(3-chloro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-74-6P, 5-Ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-3-methylphenyl)-6-methyl-3H-pyrimidin-4-one 780771-75-7P, 2-(4-Chloro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-76-8P, 5-Ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-4-methoxyphenyl)-6-methyl-3H-pyrimidin-4-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinone compds. as calcilytics)

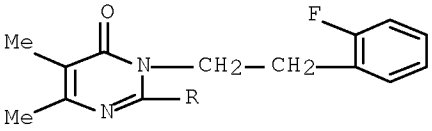
RN 780771-35-9 CAPLUS

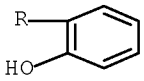
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5,6-dimethyl-3-(2-phenylethyl)-

(CA INDEX NAME)

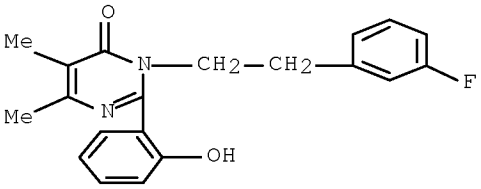


RN 780771-40-6 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl- (CA INDEX NAME)

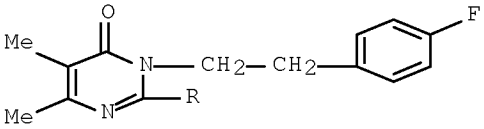


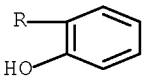


RN 780771-41-7 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl- (CA INDEX NAME)

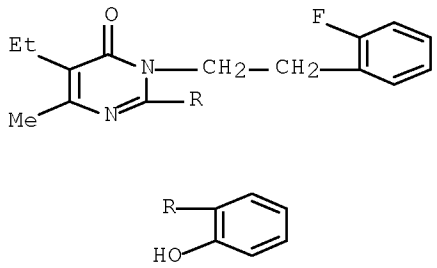


RN 780771-42-8 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(4-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl- (CA INDEX NAME)

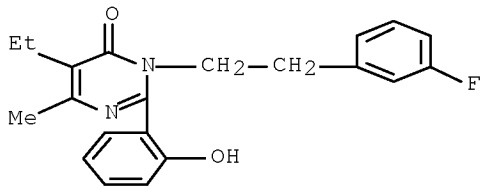




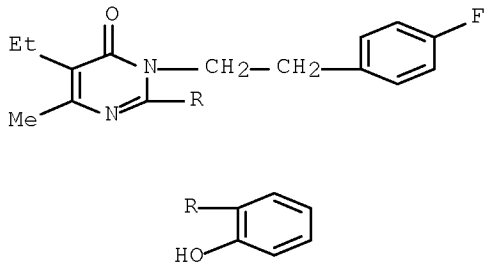
RN 780771-44-0 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



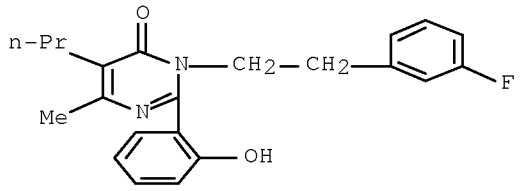
RN 780771-45-1 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



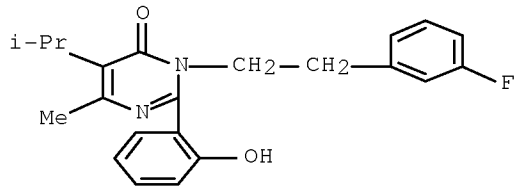
RN 780771-46-2 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(4-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



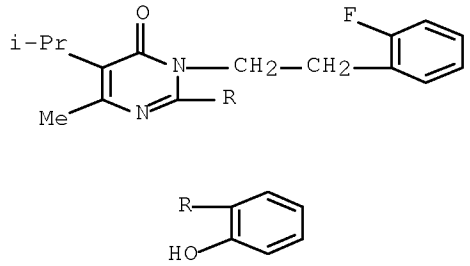
RN 780771-47-3 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-propyl- (CA INDEX NAME)



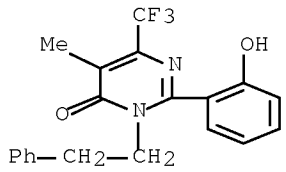
RN 780771-48-4 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



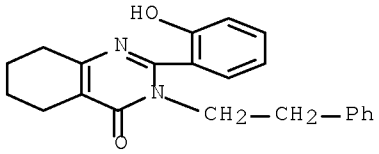
RN 780771-52-0 CAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



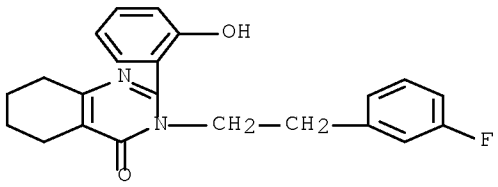
RN 780771-53-1 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5-methyl-3-(2-phenylethyl)-6-(trifluoromethyl)- (CA INDEX NAME)



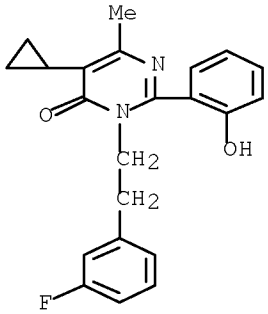
RN 780771-54-2 CAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



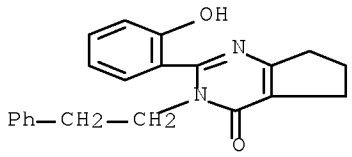
RN 780771-55-3 CAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)- (CA INDEX NAME)



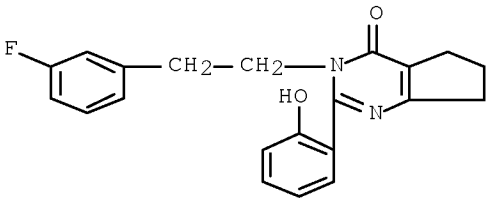
RN 780771-56-4 CAPLUS
CN 4(3H)-Pyrimidinone, 5-cyclopropyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



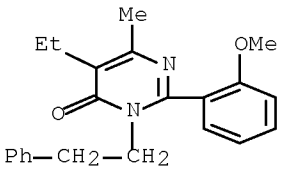
RN 780771-57-5 CAPLUS
CN 4H-Cyclopentapyrimidin-4-one, 3,5,6,7-tetrahydro-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (9CI) (CA INDEX NAME)



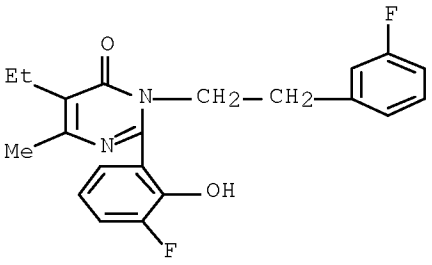
RN 780771-58-6 CAPLUS
CN 4H-Cyclopentapyrimidin-4-one, 3-[2-(3-fluorophenyl)ethyl]-3,5,6,7-tetrahydro-2-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)



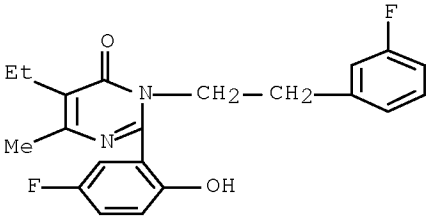
RN 780771-59-7 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-methoxyphenyl)-6-methyl-3-(2-phenylethyl)-
(CA INDEX NAME)



RN 780771-62-2 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-
fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)

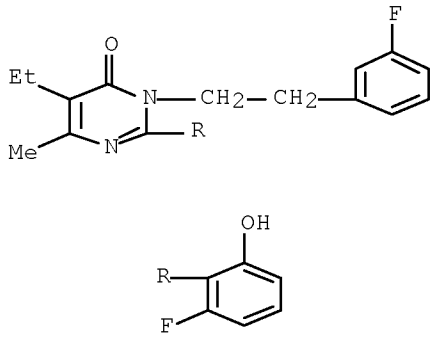


RN 780771-64-4 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(5-fluoro-2-hydroxyphenyl)-3-[2-(3-
fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



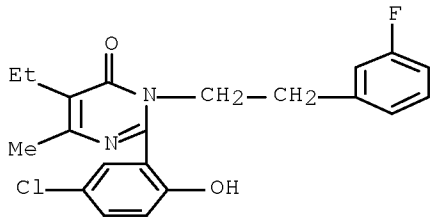
RN 780771-65-5 CAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-fluoro-6-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



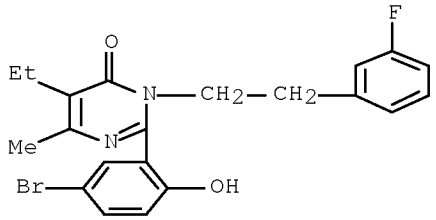
RN 780771-67-7 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(5-chloro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



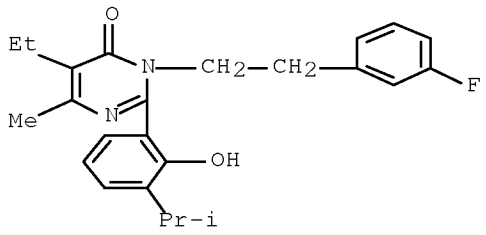
RN 780771-68-8 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(5-bromo-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)

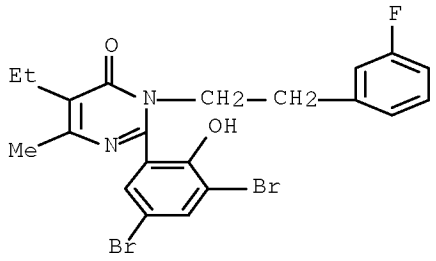


RN 780771-69-9 CAPLUS

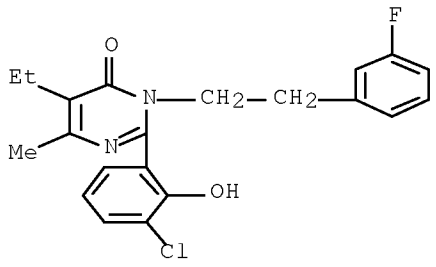
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(3-fluorophenyl)ethyl]-2-[2-hydroxy-3-(1-methylethyl)phenyl]-6-methyl- (CA INDEX NAME)



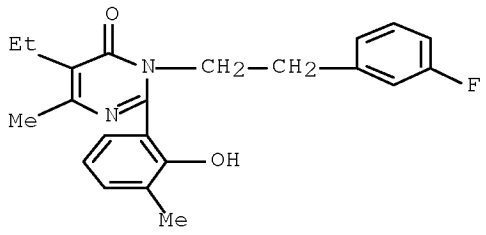
RN 780771-71-3 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3,5-dibromo-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



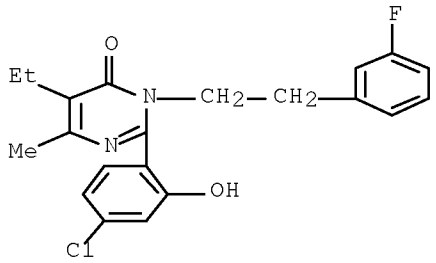
RN 780771-72-4 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-chloro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



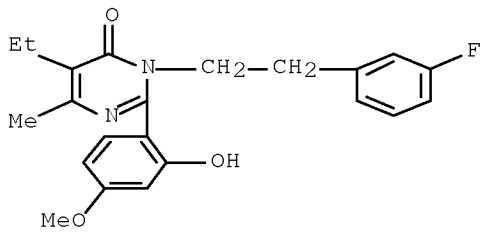
RN 780771-74-6 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-3-methylphenyl)-6-methyl- (CA INDEX NAME)



RN 780771-75-7 CAPLUS
CN 4(3H)-Pyrimidinone, 2-(4-chloro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



RN 780771-76-8 CAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-4-methoxyphenyl)-6-methyl- (CA INDEX NAME)



FILE 'HOME' ENTERED AT 14:38:47 ON 01 FEB 2008

SEARCH HISTORY

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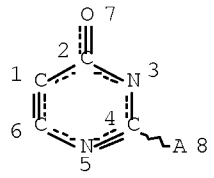
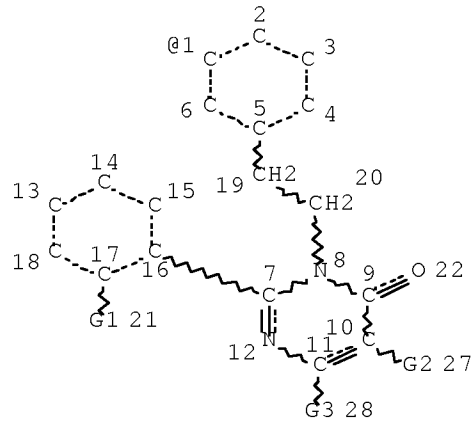
L1 STR

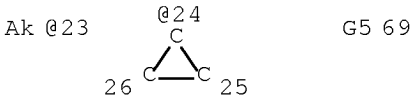


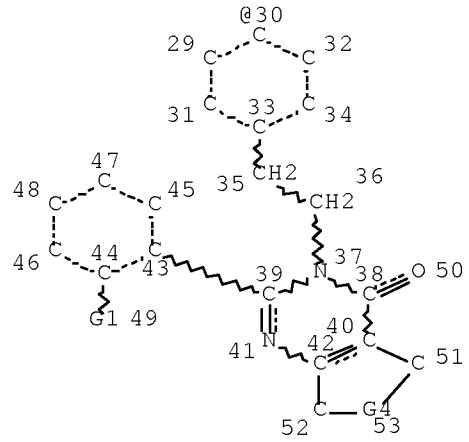
NODE ATTRIBUTES:
NSPEC IS RC AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

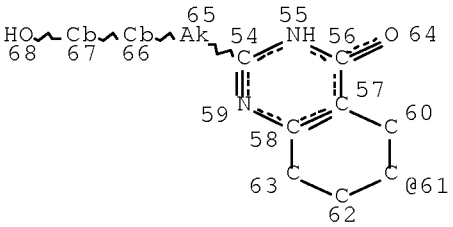
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L2 448706 SEA FILE=REGISTRY SSS FUL L1
L33 STR









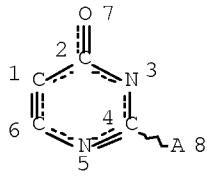
Page 2-A
VAR G1=OH/OME
VAR G2=23/24
VAR G3=23/CF3
REP G4=(1-2) C
VAR G5=1/61/30
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 23
CONNECT IS E2 RC AT 65
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY LOC UNS AT 66
GGCAT   IS MCY LOC UNS AT 67
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 69

STEREO ATTRIBUTES: NONE
L36   82 SEA FILE=REGISTRY SUB=L2 SSS FUL L33

100.0% PROCESSED   21805 ITERATIONS   82 ANSWERS
SEARCH TIME: 00.00.01

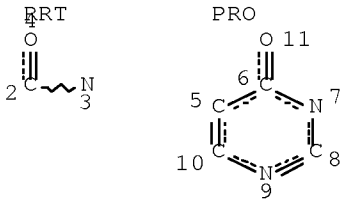
L1   STR



NODE ATTRIBUTES:
NSPEC   IS RC   AT   8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   8

STEREO ATTRIBUTES: NONE
L2   448706 SEA FILE=REGISTRY SSS FUL L1
L4   46492 SEA FILE=REGISTRY ABB=ON L2 AND CASREACT/LC
L5   10919 SEA FILE=CASREACT ABB=ON L4
L8   STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

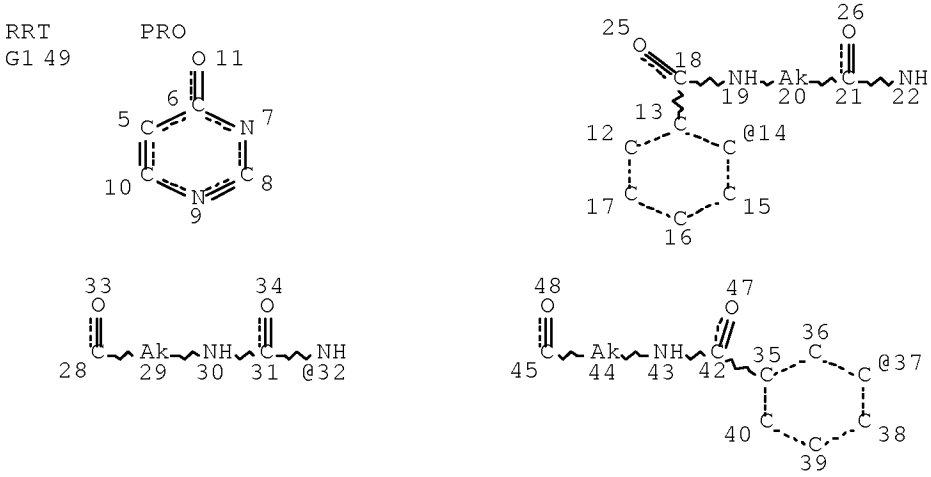
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

****MAPPINGS****

NOD	SYM	ROL	NOD	SYM	ROL
2	C	RRT	6	C	PRO
3	N	RRT	7	N	PRO
4	O	RRT	11	O	PRO
6	C	PRO	2	C	RRT
7	N	PRO	3	N	RRT
11	O	PRO	4	O	RRT

L11 1257 SEA FILE=CASREACT SUB=L5 SSS FUL L8 (11881 REACTIONS)
L12 1118 SEA FILE=CASREACT ABB=ON L11/COMPLETE
L13 902 SEA FILE=CASREACT ABB=ON L12 AND (PY<2004 OR AY<2004 OR PRY<2004)
L16 STR



VAR G1=14/32/37
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 20
CONNECT IS E2 RC AT 29
CONNECT IS E2 RC AT 44
DEFAULT MLEVEL IS ATOM

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  40

STEREO ATTRIBUTES: NONE
L19          22 SEA FILE=CASREACT SUB=L11 SSS FUL L16 (    56 REACTIONS)
L20          16 SEA FILE=CASREACT ABB=ON  L13 AND L19




     (FILE 'CAPLUS' ENTERED AT 11:20:31 ON 01 FEB 2008)
                DEL HIS Y

     FILE 'REGISTRY' ENTERED AT 12:04:27 ON 01 FEB 2008
                ACT JAI920BAT/A
               ---------
L1              STR
L2        448706 SEA SSS FUL L1
               ---------
                ACT JAI920REG/A
               ---------
L3            39 SEA ABB=ON  (116046-53-8/BI OR 128095-14-7/BI OR 1583-88-6/BI
                  OR 1655-07-8/BI OR 21615-34-9/BI OR 22396-14-1/BI OR 404-70-6/B
                  I OR 51756-10-6/BI OR 52721-69-4/BI OR 5538-51-2/BI OR
                  607-97-6/BI OR 609-14-3/BI OR 611-10-9/BI OR 64-04-0/BI OR
                  780771-35-9/BI OR 780771-36-0/BI OR 780771-37-1/BI OR 780771-38
                  -2/BI OR 780771-39-3/BI OR 780771-40-6/BI OR 780771-41-7/BI OR
                  780771-42-8/BI OR 780771-43-9/BI OR 780771-44-0/BI OR 780771-45
                  -1/BI OR 780771-46-2/BI OR 780771-47-3/BI OR 780771-48-4/BI OR
                  780771-49-5/BI OR 780771-50-8/BI OR 780771-51-9/BI OR 780771-52
                  -0/BI OR 780771-54-2/BI OR 780771-55-3/BI OR 780771-56-4/BI OR
                  780771-57-5/BI OR 780771-58-6/BI OR 85796-29-8/BI OR 916335-88-
                  1/BI)
                ---------
                 D SCAN
L4         46492 SEA ABB=ON  L2 AND CASREACT/LC

     FILE 'CASREACT' ENTERED AT 12:08:50 ON 01 FEB 2008
L5         10919 SEA ABB=ON  L4
L6               STR
L7            21 SEA SUB=L5 SSS SAM L6 (    86 REACTIONS)

     FILE 'STNGUIDE' ENTERED AT 12:13:44 ON 01 FEB 2008

     FILE 'CASREACT' ENTERED AT 12:18:01 ON 01 FEB 2008

     FILE 'STNGUIDE' ENTERED AT 12:25:43 ON 01 FEB 2008

     FILE 'CASREACT' ENTERED AT 12:29:29 ON 01 FEB 2008
L8               STR L6
L9            50 SEA SUB=L5 SSS SAM L8 (   408 REACTIONS)
L10         4853 SEA SUB=L5 SSS FUL L8 ( 71375 REACTIONS) EXTEND
L11         1257 SEA SUB=L5 SSS FUL L8 ( 11881 REACTIONS)
L12         1118 SEA ABB=ON  L11/COMPLETE
                 SAVE TEMP L12 JAI920CSRFL/A
L13          902 SEA ABB=ON  L12 AND (PY<2004 OR AY<2004 OR PRY<2004)
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     FILE 'STNGUIDE' ENTERED AT 12:32:35 ON 01 FEB 2008

     FILE 'CASREACT' ENTERED AT 12:58:34 ON 01 FEB 2008
L14             STR L6
L15           0 SEA SUB=L11 SSS SAM L14 (     0 REACTIONS)
L16             STR L14
L17           1 SEA SUB=L11 SSS SAM L16 (     1 REACTIONS)
                D SCAN
L18         870 SEA SUB=L11 SSS FUL L16 (  7481 REACTIONS) EXTEND
L19          22 SEA SUB=L11 SSS FUL L16 (    56 REACTIONS)
                SAVE TEMP L19 JAI920SUB1/A
L20          16 SEA ABB=ON  L13 AND L19
                ACT JAI920CSRAU/A
                ---------
L21 (        29)SEA ABB=ON  SHCHERBAKOVA I?/AU
L22 (         0)SEA ABB=ON  BALANDRIA M?/AU
L23 (       108)SEA ABB=ON  HUANG G?/AU
L24 (         5)SEA ABB=ON  GEOFFROY O?/AU
L25 (       117)SEA ABB=ON  FOX J?/AU
L26 (        51)SEA ABB=ON  NAIR S?/AU
L27 (         7)SEA ABB=ON  BALANDRIN M?/AU
L28           4 SEA ABB=ON  (L21 AND (L22 OR L23 OR L24 OR L25 OR L26 OR L27))
                OR (L23 AND (L24 OR L25 OR L26 OR L27)) OR (L24 AND (L25 OR
                L26 OR L27)) OR (L25 AND (L26 OR L27)) OR (L26 AND L27)
                ---------
L29           4 SEA ABB=ON  L28 OR (L28 AND L11)

     FILE 'REGISTRY' ENTERED AT 14:09:44 ON 01 FEB 2008
L30             STR
L31          12 SEA SUB=L2 SSS SAM L30

     FILE 'ZCAPLUS' ENTERED AT 14:14:18 ON 01 FEB 2008
L32           2 SEA ABB=ON  L31
                D SCA TI

     FILE 'REGISTRY' ENTERED AT 14:16:04 ON 01 FEB 2008
L33             STR
L34           2 SEA SUB=L2 SSS SAM L33
                D SCAN
L35       21805 SEA SUB=L2 SSS FUL L33 EXTEND
L36          82 SEA SUB=L2 SSS FUL L33
                SAVE TEMP L36 JAI920SUB2/A

     FILE 'CAPLUS' ENTERED AT 14:29:07 ON 01 FEB 2008
L37           5 SEA ABB=ON  L36/P
                D SCAN TI
                ACT JAI920CAAU/A
                ---------
L38           1 SEA ABB=ON  US2006-551920/AP
                ---------
L39           1 SEA ABB=ON  L38 AND L37
                D SCAN

     FILE 'CASREACT' ENTERED AT 14:31:11 ON 01 FEB 2008

     FILE 'CAPLUS' ENTERED AT 14:33:03 ON 01 FEB 2008
L40       12524 SEA ABB=ON  L3
L41           1 SEA ABB=ON  L40 AND L38
                D QUE NOS L41
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     FILE 'CASREACT' ENTERED AT 14:34:13 ON 01 FEB 2008
                D QUE NOS L29

     FILE 'CAPLUS, CASREACT' ENTERED AT 14:34:22 ON 01 FEB 2008
L42              4 DUP REM L41 L29 (1 DUPLICATE REMOVED)
                       ANSWER '1' FROM FILE CAPLUS
                       ANSWERS '2-4' FROM FILE CASREACT
                D IBIB ABS HITSTR 1
                D IBIB ABS IND 3-4

     FILE 'CASREACT' ENTERED AT 14:36:57 ON 01 FEB 2008

     FILE 'CASREACT, CAPLUS' ENTERED AT 14:37:06 ON 01 FEB 2008
                D IBIB ABS IND 3-4

     FILE 'CASREACT' ENTERED AT 14:37:07 ON 01 FEB 2008

     FILE 'CASREACT' ENTERED AT 14:37:44 ON 01 FEB 2008
                D STAT QUE L20
L43             14 SEA ABB=ON  L20 NOT L29

     FILE 'REGISTRY' ENTERED AT 14:37:45 ON 01 FEB 2008
                D STAT QUE L36

     FILE 'CAPLUS' ENTERED AT 14:37:45 ON 01 FEB 2008
                D QUE NOS L37
L44              4 SEA ABB=ON  L37 NOT L41

     FILE 'CASREACT, CAPLUS' ENTERED AT 14:38:00 ON 01 FEB 2008
L45             18 DUP REM L43 L44 (0 DUPLICATES REMOVED)
                       ANSWERS '1-14' FROM FILE CASREACT
                       ANSWERS '15-18' FROM FILE CAPLUS
                D IBIB ABS FHIT 1-14
                D IBIB ABS HITSTR 15-18

     FILE 'HOME' ENTERED AT 14:38:47 ON 01 FEB 2008
                D STAT QUE L36
                D STAT QUE L20

=>
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